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CRYSTALLIZATION AND STRUCTURE OF *STAPHYLOCOCCUS AUREUS* PEPTIDE DEFORMYLASE

This application claims the benefit of the U.S. Provisional Application Serial No. 60/215,550, filed June 30, 2000, which is incorporated herein by reference in its entirety.

FIELD OF THE INVENTION

The present invention is related to the crystallization and structure determination of *Staphylococcus aureus* peptide deformylase (*S. aureus* pdf).

BACKGROUND OF THE INVENTION

In all bacteria as well as mitochondria and chloroplasts the initiation of protein synthesis normally requires an N-formylated methionine residue. The special initiation tRNA, $tRNA_f^{Met}$, is charged with methionine by the Methionyl-tRNA synthetase (EC 6.1.10) which adds a methionine to either of the methionine tRNAs with the consumption of ATP. The formyl group is added to the charged $tRNA_f^{Met}$ from 10-formyltetrahydrofolate which is catalyzed by methionine-$tRNA_f^{Met}$ formyl-transferase (EC 2.1.2.9). The formylated tRNA is transferred to the ribosome where protein synthesis is initiated (Figure 1). All nascent polypeptides are synthesized with N-formyl methionine at the n-terminus.

Mature proteins do not by and large retain n-formyl methionine at the n-terminus. In fact, a rather heterogenous population of amino acids are normally found at the n-terminus of mature proteins---alanine, glycine, serine, threonine, or methionine. Larger amino acids are rarely found, which suggests that multiple catabolic processing might occur after or in concert with protein synthesis. All known amino-terminal peptidases cannot use formylated peptides as substrates. After translation, the formyl group is removed by Peptide Deformylase (pdf) as illustrated in Figure 2. This metalloenzyme (EC 3.5.1.27) removes the formyl group from the peptide amino-terminus and releases the protein for possible further processing by methionine aminopeptidase (MAP; EC 3.4.11.18). The formylation/deformylation cycle is unique to eubacteria and does not occur in eucaryotic protein synthesis. The essential deformylation activity of pdf makes it an attractive target for crystallization and structural studies. Such studies may lead to the design of new antibiotics.

SUMMARY OF THE INVENTION

In one aspect, the present invention provides crystalline *S. aureus* peptide deformylase. Optionally, one or more methionine may be replaced with selenomethionine. The crystal may optionally include a coordinated metal ion selected from the group of metals consisting of Fe, Zn, Ni and combinations thereof.

In one embodiment, the crystal has the orthorhombic space group symmetry $C222_1$. Preferably, the unit cell has dimensions a, b, and c; wherein a is about 90 Å to about 100 Å, b is about 116 Å to about 128 Å, and c is about 45 Å to about 50 Å; and wherein $\alpha = \beta = \gamma = 90°$. More preferably, a is about 92 Å to about 95 Å, b is about 121 Å to about 124 Å, and c is about 47 Å to about 49 Å.

In another embodiment, the present invention provides a crystal of *S. aureus* peptide deformylase having the monoclinic space group symmetry C2. Preferably, the unit cell has dimensions a, b, and c; wherein a is about 85 Å to about 100 Å, b is about 35 Å to about 50 Å, and c is about 90 Å to about 110 Å; and wherein $\alpha = \gamma = 90°$ and β is about 90° to about 95°. More preferably, a is about 91 Å to about 95 Å, b is about 41 Å to about 44 Å, and c is about 102 Å to about 105 Å.

In still another embodiment, the present invention provides a crystal of *S. aureus* peptide deformylase having the tetragonal space group symmetry $P4_1$ or $P4_22_12$. Preferably, the unit cell has dimensions a, b, and c; wherein a and b are about 130 Å to about 190 Å, and c is about 30 Å to about 70 Å; and wherein $\alpha=\beta = \gamma = 90°$. More preferably, a and b are about 160 Å to about 164 Å, and c is about 45 Å to about 49 Å.

In another aspect, the present invention provides a method for crystallizing an *S. aureus* peptide deformylase molecule or molecular complex. In one embodiment the method includes preparing a stock solution of purified *S. aureus* peptide deformylase at a concentration of about 1 mg/ml to about 50 mg/ml; contacting the stock solution with a precipitating solution containing about 1 % by weight to about 35 % by weight PEG having a number average molecular weight between about 300 and about 20,000; about 0 M to about 0.2 M $MgCl_2$; and about 0 % by weight to about 25 % by weight DMSO; the precipitating solution being buffered to a pH of about 5 to about 9; and allowing *S. aureus* peptide deformylase to crystallize from the resulting solution. Preferably, the precipitating solution contains about 15 % by weight to about 25 % by weight PEG having a number average molecular weight between about 3000 and about 5,000; about 0.05 M to about 0.15 M $MgCl_2$ and is buffered to a pH of about 8 to about 9.

In another embodiment the method for crystallizing an *S. aureus* peptide deformylase molecule or molecular complex includes preparing a stock solution of purified *S. aureus* peptide deformylase at a concentration of about 1 mg/ml to about 50 mg/ml; contacting the stock solution with a precipitating solution containing

about 1 % by weight to about 40 % by weight PEG having a number average molecular weight between about 300 and about 20,000; about 0.005 M to about 0.5 M citric acid; about 0 % by weight to about 25 % by weight DMSO; and sufficient base to adjust the pH of the precipitating solution to about 5.0 to about 6.5; and allowing *S. aureus* peptide deformylase to crystallize from the resulting solution. Preferably, the precipitating solution contains about 1 % by weight to about 40 % by weight PEG having a number average molecular weight between about 2000 and about 4,000; about 0.05 M to about 0.2 M citric acid, and sufficient base to adjust the pH of the precipitating solution to about 5.0 to about 5.5.

In still another embodiment the method for crystallizing an *S. aureus* peptide deformylase molecule or molecular complex includes preparing a stock solution of purified *S. aureus* peptide deformylase at a concentration of about 1 mg/ml to about 50 mg/ml; contacting the stock solution with a precipitating solution containing about 0.2 M to about 1.5 M sodium citrate; about 0.005 M to about 0.5 M Hepes; about 0 % by weight to about 25 % by weight DMSO; and sufficient base to adjust the pH of the precipitating solution to about 7.0 to about 8.5; and allowing *S. aureus* peptide deformylase to crystallize from the resulting solution. Preferably, the precipitating solution contains about 25 % by weight to about 35 % by weight PEG having a number average molecular weight between about 2000 and about 4,000; about 0.05 M to about 0.2 M citric acid, and sufficient base to adjust the pH of the precipitating solution to about 5.0 to about 5.5.

In still another embodiment the method for crystallizing an *S. aureus* peptide deformylase molecule or molecular complex includes preparing a stock solution of purified *S. aureus* peptide deformylase at a concentration of about 1 mg/ml to about 50 mg/ml; contacting the stock solution with a precipitating solution containing about 1 % by weight to about 40 % by weight PEG having a number average molecular weight between about 300 and about 20,000; about 0 M to about 0.4 M $MgCl_2$; and about 0 % by weight to about 25 % by weight DMSO; the precipitating solution being buffered to a pH of about 7 to about 9; and

allowing *S. aureus* peptide deformylase to crystallize from the resulting solution. Preferably, the precipitating solution contains about 15 % by weight to about 35 % by weight PEG having a number average molecular weight between about 3,000 and about 5,000; about 0.05 M to about 0.3 M $MgCl_2$; and the precipitating solution being buffered to a pH of about 8 to about 9.

In another aspect, the present invention provides a molecule or molecular complex including at least a portion of an *S. aureus* peptide deformylase or an *S. aureus* peptide deformylase-like active site including amino acids Gly58, Gly60, Leu61, Gln65, Glu109 , Gly110, Cys111, Leu112, Ile150, His154, Glu155, and His158, the active site being defined by a set of points having a root mean square deviation of less than about 0.35 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1. Optionally, the molecule or molecular complex further includes a coordinated metal ion selected from the group of metals consisting of Fe, Zn, Ni and combinations thereof. Preferably, the metal ion is coordinated by the amino acids Cys111, His154, and His158.

In another aspect, the present invention provides a scalable three-dimensional configuration of points, at least a portion of said points, and preferably all of said points, derived from structure coordinates of at least a portion of an *S. aureus* peptide deformylase molecule or molecular complex listed in Table 1 and having a root mean square deviation of less than about 1.4 Å from said structure coordinates. Preferably, at least a portion of the points are derived from the *S. aureus* peptide deformylase structure coordinates are derived from structure coordinates representing the locations of at least the backbone atoms of a plurality of the amino acids defining at least one *S. aureus* peptide deformylase or *S. aureus* peptide deformylase-like active site, the active site including amino acids Gly58, Gly60, Leu61, Gln65, Glu109 , Gly110, Cys111, Leu112, Ile150, His154, Glu155, and His158.

In another aspect, the present invention provides a machine-readable data storage medium including a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, displays a graphical three-dimensional representation of at least one molecule or molecular complex selected from the group consisting of (i) a molecule or molecular complex including at least a portion of an *S. aureus* peptide deformylase or an *S. aureus* peptide deformylase-like active site including amino acids Gly58, Gly60, Leu61, Gln65, Glu109 , Gly110, Cys111, Leu112, Ile150, His154, Glu155, and His158, the active site being defined by a set of points having a root mean square deviation of less than about 0.35 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

In another aspect, the present invention provides a computer-assisted method for obtaining structural information about a molecule or a molecular complex of unknown structure including: crystallizing the molecule or molecular complex; generating an x-ray diffraction pattern from the crystallized molecule or molecular complex; applying at least a portion of the structure coordinates set forth in Table 1 to the x-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown.

In another aspect, the present invention provides a computer-assisted method for homology modeling an *S. aureus* peptide deformylase homolog including: aligning the amino acid sequence of an *S. aureus* peptide deformylase homolog with the amino acid sequence of *S. aureus* peptide deformylase SEQ ID NO:1 and incorporating the sequence of the *S. aureus* peptide deformylase homolog into a model of *S. aureus* peptide deformylase derived from structure coordinates set forth in Table 1 to yield a preliminary model of the *S. aureus* peptide deformylase homolog; subjecting the preliminary model to energy minimization to yield an energy minimized model; remodeling regions of the energy minimized

model where stereochemistry restraints are violated to yield a final model of the *S. aureus* peptide deformylase homolog.

In another aspect, the present invention provides a computer-assisted method for identifying a potential modifier of *S. aureus* peptide deformylase activity including: supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex including at least a portion of at least one *S. aureus* peptide deformylase or *S. aureus* peptide deformylase-like active site, the active site including amino acids Gly58, Gly60, Leu61, Gln65, Glu109 , Gly110, Cys111, Leu112, Ile150, His154, Glu155, and His158; supplying the computer modeling application with a set of structure coordinates of a chemical entity; and determining whether the chemical entity is expected to bind to the molecule or molecular complex, wherein binding to the molecule or molecular complex is indicative of potential modification of *S. aureus* peptide deformylase activity.

In another aspect, the present invention provides a computer-assisted method for designing a potential modifier of *S. aureus* peptide deformylase activity including: supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex including at least a portion of at least one *S. aureus* peptide deformylase or *S. aureus* peptide deformylase-like active site, the active site including amino acids Gly58, Gly60, Leu61, Gln65, Glu109 , Gly110, Cys111, Leu112, Ile150, His154, Glu155, and His158; supplying the computer modeling application with a set of structure coordinates for a chemical entity; evaluating the potential binding interactions between the chemical entity and active site of the molecule or molecular complex; structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and determining whether the modified chemical entity is expected to bind to the molecule or molecular complex, wherein binding to the molecule or molecular complex is indicative of potential modification of *S. aureus* peptide deformylase activity.

In another aspect, the present invention provides a computer-assisted method for designing a potential modifier of *S. aureus* peptide deformylase activity *de novo* including: supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex including at least a portion of at least one *S. aureus* peptide deformylase or *S. aureus* peptide deformylase-like active site, wherein the active site includes amino acids Gly58, Gly60, Leu61, Gln65, Glu109 , Gly110, Cys111, Leu112, Ile150, His154, Glu155, and His158; forming a chemical entity represented by set of structure coordinates; and determining whether the chemical entity is expected to bind to the molecule or molecular complex, wherein binding to the molecule or molecular complex is indicative of potential modification of *S. aureus* peptide deformylase activity.

In another aspect, the present invention provides a method for making a potential modifier of *S. aureus* peptide deformylase activity, the method including chemically or enzymatically synthesizing a chemical entity to yield a potential modifier of *S. aureus* peptide deformylase activity, the chemical entity having been identified during a computer-assisted process including supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex including at least a portion of a *S. aureus* peptide deformylase or *S. aureus* peptide deformylase-like active site; supplying the computer modeling application with a set of structure coordinates of a chemical entity; and determining whether the chemical entity is expected to bind to the molecule or molecular complex at the active site, wherein binding to the molecule or molecular complex is indicative of potential modification of *S. aureus* peptide deformylase activity.

In another aspect, the present invention provides a method for making a potential modifier of *S. aureus* peptide deformylase activity, the method including chemically or enzymatically synthesizing a chemical entity to yield a potential modifier of *S. aureus* peptide deformylase activity, the chemical entity having been

designed during a computer-assisted process including supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex including at least a portion of a *S. aureus* peptide deformylase or *S. aureus* peptide deformylase-like active site; supplying the computer modeling application with a set of structure coordinates for a chemical entity; evaluating the potential binding interactions between the chemical entity and the active site of the molecule or molecular complex; structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and determining whether the chemical entity is expected to bind to the molecule or molecular complex at the active site, wherein binding to the molecule or molecular complex is indicative of potential modification of *S. aureus* peptide deformylase activity.

In another aspect, the present invention provides a method for making a potential modifier of *S. aureus* peptide deformylase activity, the method including chemically or enzymatically synthesizing a chemical entity to yield a potential modifier of *S. aureus* peptide deformylase activity, the chemical entity having been designed during a computer-assisted process including supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex including at least a portion of a *S. aureus* peptide deformylase or *S. aureus* peptide deformylase-like active site; forming a chemical entity represented by set of structure coordinates; and determining whether the chemical entity is expected to bind to the molecule or molecular complex at the active site, wherein binding to the molecule or molecular complex is indicative of potential modification of *S. aureus* peptide deformylase activity.

Table 1 lists the atomic structure coordinates for molecule *Staphylococcus aureus* peptide deformylase (*S. aureus* pdf) as derived by x-ray diffraction from a crystal of the protein. The following abbreviations are used in Table 1:

"Atom type" refers to the element whose coordinates are measured. The first letter in the column defines the element.

"X, Y, Z" crystallographically define the atomic position of the element measured.

"B" is a thermal factor that measures movement of the atom around its atomic center.

"Occ" is an occupancy factor that refers to the fraction of the molecules in which each atom occupies the position specified by the coordinates. A value of "1" indicates that each atom has the same conformation, i.e., the same position, in all molecules of the crystal.

ABBREVIATIONS

The following abbreviations are used throughout this disclosure:

Staphylococcus aureus (*S. aureus*)

Escherichia coli (*E. coli*)

Haemophilis influenzae (*Haemop. influenzae*)

Bacillus subtilis (*B. subtilis*)

Mycoplasma pneumoniae (*Mycopl. pneumoniae*)

Peptide deformylase (pdf)

Isopropylthio-β-D-galactoside (IPTG)

(S)-2-O-(H-phosphonoxy)-L-caproyl-L-leucyl-p-nitroanilide (PCLNA)

Dimethyl sulfoxide (DMSO)

Polyethylene glycol (PEG)

Beta-mercaptoethanol (BME)

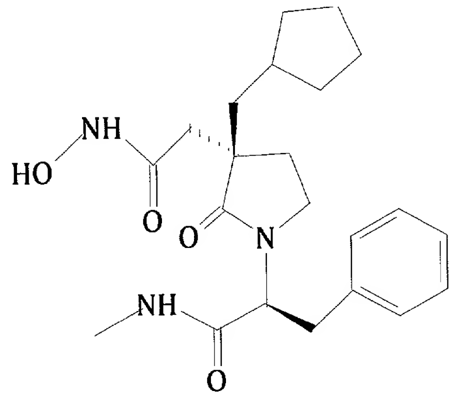
Optical density (OD)

Multiple anomalous dispersion (MAD)

Root mean square (r.m.s.)

Root mean square deviation (r.m.s.d.)

PNU-172550 is a compound having the following structure:



The following abbreviations are used for amino acids throughout this disclosure:

A = Ala = Alanine	T = Thr = Threonine
V = Val = Valine	C = Cys = Cysteine
L = Leu = Leucine	Y = Tyr = Tyrosine
I = Ile = Isoleucine	N = Asn = Asparagine
P = Pro = Proline	Q = Gln = Glutamine
F = Phe = Phenylalanine	D = Asp = Aspartic Acid
W = Trp = Tryptophan	E = Glu = Glutamic Acid
M = Met = Methionine	K = Lys = Lysine
G = Gly = Glycine	R = Arg = Arginine
S = Ser = Serine	H = His = Histidine

BRIEF DESCRIPTION OF THE FIGURES

Figure 1 is a schematic representation of the methionine cycle in bacteria.

Figure 2 is a schematic representation of the reaction catalyzed by peptide deformylase.

Figure 3 lists the amino acid sequences of peptide deformylases from various species of bacteria including *Staphylococcus aureus* peptide deformylase (pdf) with C-terminal 6xHis tag (SEQ ID NO: 1); *Escherichia coli* pdf (SEQ ID NO:2); *Haemophilis influenzae* pdf (SEQ ID NO:3); *Bacillus subtilis* (SEQ ID NO:4); and *Mycoplasma pneumoniae* (SEQ ID NO:5); and *Staphylococcus aureus* defl gene (a related but inactive form of the protein, also called Pseudo pdf) (SEQ ID NO:6). Alignments were generated from GCG SeqLab (Wisconsin Package Version 10.1, Genetics Computer Group, Madision, WI). The underlined residues show regions of importance to the activity of peptide deformylases. The highlighted amino acids show mutations for *S. aureus* pdf (SEQ ID NO:1).

Figure 4 is a photograph illustrating 4-20% SDS PAGE gel of pseudo pdf, pdf1, and further purified pdf2.

Figure 5 is a schematic secondary structure diagram of *S. aureus* pdf.

Figure 6 is a depiction of the secondary structure of *S. aureus* peptide deformylase. The α-helices are starred and the β-sheets are not starred. Random coil connections are light gray. The single Zn/Fe atom is labeled **.

Figure 7 is a stereo pair view of *S. aureus* peptide deformylase backbone from the same view as in Figure 6.

Figure 8 is a model showing the electro-static surface potential for pdf. The positively charged region is indicated by the arrow (+100 kcal) while the negatively charged regions are gray (-100 kcal). The surface potential was created in MOSAIC2 (Computer Aided Drug Discovery) using point charge parameters derived from the AMBER force field (Weiner et al., *J. Comput. Chem.*, 7:230-52 (1986)) and a formal charge of plus 2 for the metal ion.

Figure 9 is a schematic model showing the active site metal ion (gray sphere). The metal ion may be Zn, Ni, or Fe. The ion is coordinated by protein sidechains H154, H158 and C111.

Figure 10 is a sequence alignment based on x-ray structure comparisons for *E. coli* pdf and *S. aureus* pdf proteins.

Figure 11 is a depiction of the secondary structure of pdf for a) *S. aureus* pdf and b) *E. coli* pdf. The n-terminus ends are starred.

Figure 12 is a stereo pair view of the superimposed alpha carbons from *S. aureus* pdf (dark) and *E. coli* pdf (light). The metal ion is indicated by the sphere.

Figure 13 is a stereo pair view of the superposition of the active site cavity of the *E. coli* pdf structure. Some selected residues from *S. aureus* pdf are labeled.

Figure 14 a) is a schematic illustration of PCLNA inhibitor (Hao et al., *Biochemistry*, 38: 4712-19 (1999)) placing subsituents into three pdf subsites. The *S. aureus* residue number is given first with the equivalent *E. coli* amino acid subsequent. The metal ion is the labeled sphere. Figure 14 b) is a view of a surface rendering for the PCLNA complex with the *E. coli* enzyme with the location of the subsites indicated. The light gray surface represents hydrophobic surface associated with carbon atoms, dark gray for nitrogen atoms and medium gray for oxygen atoms.

Figure 15 is a view of a model of the active site cleft of *S. aureus* pdf with PCLNA (from Hao et al., *Biochemistry*, 38: 4712-19 (1999)). The surface is colored according to atom type with all carbons in light gray, oxygens in medium gray, and nitrogens in dark gray. The six active site residues which are conserved between *E. coli* and *S. aureus* pdf are indicated in white. These residues line the bottom of the active site.

Figure 16 is a view of a model of the surface rendering for PCLNA complex with *E. coli* enzyme (left) and of PCLNA with *S. aureus* enzyme (right). The light gray colors indicate the hydrophobic surface associated with carbon atoms, dark gray is for nitrogen atoms, and medium gray for oxygen atoms. Amino acid labeling indicates the surface corresponding to various residues.

Figure 17 is a stereo view of the S1 subsite of pdf with PCLNA inhibitor. The amino acid sidechains which surround the P1, caproyl group, are indicated. Labels indicate the *S.aureus* amino acid first and the equivalent *E.coli* residue second. However, R97/N is indicated with the opposite nomenclature.

Figure 18 is a stereo view of the S2 subsite of pdf with PCLNA inhibitor. The amino acid sidechains which surround the P2, leucyl group, are indicated. Labels indicate the *S.aureus* amino acid first and the equivalent *E.coli* residue second. However, R97/N is indicated with the opposite nomenclature.

Figure 19 is a stereo view of the S3 subsite of pdf with PCLNA inhibitor. The amino acid sidechains which surround the P3, p-nitroanilide group, are indicated. Labels indicate the *S.aureus* amino acid first and the equivalent *E.coli* residue second.

DETAILED DESCRIPTION OF THE INVENTION

$C222_1$ Space Group Crystals

In one embodiment, crystals of *S.aureus* pdf have been obtained and belong to the $C222_1$ orthorhombic space group. Crystals were grown in four conditions, but crystals used for the structure solution were grown from 20% PEG 4000, 0.1M Tris pH=8.5 and 0.1M $MgCl_2$. Se-methionine pdf crystals were also grown and data was used to solve the pdf structure. Variation in buffer and buffer pH as well as other additives such as PEG is apparent to those skilled in the art and may result in similar crystals.

The *S. aureus* pdf protein was over-expressed and purified from *E.coli*. Crystallization attempts using pdf purified only by affinity Ni-NTA chromatography did not yield crystals, but the addition of an anion exchange purification step improved results. This further purified material resulted in many promising crystallization leads including four unique hits. Each of these hits were followed up using finely focused grid screens. All four conditions were pursued and characterized according to crystal behavior and quality. All small crystals were optimized though micro-seeding. Large, single crystals suitable for data collection were soaked in stabilization solution containing 25% glycerol prior to freezing for

low temperature data collection. The useful crystals grown from the four diverse starting conditions all belong to the space group $C222_1$ with one molecule in the asymmetric unit. The unit cell parameters were a=94.1 b= 121.87 c= 47.58 Å.

Identical crystals of pdf were grown with Se-methionine pdf protein. One crystal was grown from 20% PEG 4000, 0.1M Tris pH=8.5 and 0.1m $MgCl_2$ and measured 0.22x0.22x0.6 micrometer. Data from this crystal was collected at the IMCA synchrotron facility and was found to belong to the space group $C222_1$ as well. The pdf structure was solved using this MAD data. However, the resulting structure could not be completely refined with the MAD data; so refinement was abandoned in favor of a new data set (see below).

A second crystal was grown in the presence of 2mM of a potential inhibitor, 10% DMSO, 20% PEG 4000, 0.1M Tris pH=8.5 and 0.1M $MgCl_2$. This crystal measured 0.28x0.28x0.98 micrometer. No evidence for this compound was observed in the electron density map. After freezing the crystal, data was collected on a Siemens dual Hi-star. The crystal diffracted to 1.9 Å and molecular replacement was successfully performed using the MAD-derived model. This structure was refined to a final R-factor of 18.62%.

The orthorhombic crystal form could be prepared with or without compounds. The crystals belonging to the $C222_1$ space group generally have unit cell parameters with a=91.6 to 95.1 Å; b=121.3 to 123.5 Å; and c=47.6 to 48.4 Å. Crystals may be grown at 20°C, for example, by mixing a buffered protein sample with 19% PEG4000, 0.1M Tris pH 8.5 and 0.2M $MgCl_2$. Crystals may be stabilized in 25% PEG4000; 10% glycerol; 0.1M Tris pH 8.5 and 0.2M $MgCl_2$ for data collection.

C2 Space Group Crystals

The Monoclinic crystal form of *S. aureus* pdf, C2, with unit cell parameters ranging from a= 90.8 to 95.1 Å; b=42.4 to 42.7 Å; and c=104.1 to 104.4 Å. Crystals were grown at 20°C by mixing a buffered protein sample that included

5mM PNU-172550 with an equal volume of 30% PEG 3000; 0.1M Na Citrate pH 5.2. Other compounds could be crystallized using the same procedure with variation in PEG concentration or pH. Crystals were stabilized in a solution containing PEG; Citrate, PNU-172550 and 10% glycerol for diffraction studies.

$P4_22_12$ Space Group Crystals

Another crystal form could also be prepared with PNU-172550. This tetragonal crystal form $P4_22_12$ has unit cell parameters ranging from a=b=160.4 to 163.5 Å and c=45.2 to 48.3 Å. Crystals are grown at 20°C by mixing a buffered protein sample that included 5mM PNU-172550 with an equal volume of 1.375 M Na Citrate and 0.1 M Na Hepes pH 7.5. Other compounds could be crystallized using the same procedure with variation in salts and buffers. Most often no stabilization solution was employed.

Comparision of S. aureus pdf and E. coli pdf crystals

A number of structure determination reports have reported the crystallization of the pdf from *E.coli* as shown in Table 2. The present disclosure is believed to be the first crystallization of *S.aureus* pdf, and the reported crystal forms are also unique.

TABLE 2: The Space group and unit cell parameters for a variety of *E. coli* pdf crystals.

PDB No.	Space Group	A edge	B edge	C edge	Beta angle	A.U.
1bs4	$C2_1$	140.70	63.30	86.8	120.6	3
1bs5	$C2_1$	143.4	64.10	84.6	123.2	3
1bs6	$C2_1$	143.8	64.10	85.10	123.3	3
1bs7	$C2_1$	143.4	64.0	84.50	123.0	3
1bs8	$C2_1$	143.1	64.2	84.7	123.3	3
1bsz	$C2_1$	141.0	63.4	86.8	120.6	3
1dff	$P6_122$	55.35	55.35	230.92	120	1
1icj	$C2_1$	140.7	63.4	86.9	120.6	3
1bsj	$P6_522$	98.38	98.38	109.37	120	1
1bsk	$P6_522$	100.11	100.11	111.34	120	1

X-ray Crystallographic Analysis

Each of the constituent amino acids of *S. aureus* pdf is defined by a set of structure coordinates as set forth in Table 1. The term "structure coordinates" refers to Cartesian coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of x-rays by the atoms (scattering centers) of an *S. aureus* pdf complex in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are then used to establish the positions of the individual atoms of the *S. aureus* pdf protein or protein/ligand complex.

Slight variations in structure coordinates can be generated by mathematically manipulating the *S. aureus* pdf or *S. aureus* pdf/ligand structure coordinates. For example, the structure coordinates set forth in Table 1 could be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates or any combination of the above. Alternatively, modifications in the crystal structure due

to mutations, additions, substitutions, and/or deletions of amino acids, or other changes in any of the components that make up the crystal, could also yield variations in structure coordinates. Such slight variations in the individual coordinates will have little effect on overall shape. If such variations are within an acceptable standard error as compared to the original coordinates, the resulting three-dimensional shape is considered to be structurally equivalent. Structural equivalence is described in more detail below.

It should be noted that slight variations in individual structure coordinates of the *S. aureus* pdf or *S. aureus* pdf/ligand complex, as defined above, would not be expected to significantly alter the nature of ligands that could associate with the active sites. Thus, for example, a ligand that bound to the active site of *S. aureus* pdf would also be expected to bind to or interfere with another active site whose structure coordinates define a shape that falls within the acceptable error.

Binding Pockets/Active Sites/Other Structural Features

The present invention has provided, for the first time, information about the shape and structure of the active site of *S. aureus* pdf.

Active sites are of significant utility in fields such as drug discovery. The association of natural ligands or substrates with the active sites of their corresponding receptors or enzymes is the basis of many biological mechanisms of action. Similarly, many drugs exert their biological effects through association with the active sites of receptors and enzymes. Such associations may occur with all or any parts of the active site. An understanding of such associations helps lead to the design of drugs having more favorable associations with their target, and thus improved biological effects. Therefore, this information is valuable in designing potential modifiers of *S. aureus* pdf-like activity, as discussed in more detail below.

The term "active site (or binding pocket)," as used herein, refers to a region of a molecule or molecular complex, that, as a result of its shape, favorably associates with another chemical entity or compound. Thus, an active site may

include or consist of features such as interfaces between domains. Chemical entities or compounds that may associate with an active site include, but are not limited to, cofactors, substrates, inhibitors, agonists, antagonists, etc.

The active site of *S. aureus* peptide deformylase may be represented by the amino acids in the following table, which are believed would fall within 5 Å of an incorporated modifier. Using structure coordinates of *E. coli* pdf with bound PCLNA and the present *S. aureus* pdf, the structures were superimposed using the Pharmacia program SUPERPDB.

In Model A, the 12 residues that are identical between *E. coli* pdf and *S. aureus* pdf were superimposed and chosen as the set to be minimized. The resulting distances between the α-Cs for the 12 residues, and the RMS for all the atoms in each of the corresponding residues were calculated and are reported in Table 3.

In Model B, the three residues which coordinate the metal atom (Cys111, His154, and His158 for *S. aureus* pdf) were chosen as the set to be minimized, and other residues within 2 Å were brought into the refinement. The resulting distances between the α-Cs for 18 active site amino acids and the RMS for all the atoms in each of the corresponding residues were calculated and are reported in Table 3.

In Model C, the 12 residues that are identical between *E. coli* pdf and *S. aureus* pdf were chosen as the set to be minimized, and other residues within 2 Å were brought into the refinement. The distances between the α-Cs for 18 active site amino acids and the RMS for all the atoms in each of the corresponding residues were calculated and are reported in Table 3.

TABLE 3: Active Site Residues

S. aureus	*E. coli*	Model A		Model B		Model C	
		α-C Dist., Å	RMS (all atoms)	α-C Dist., Å	RMS (all atoms)	α-C Dist., Å	RMS (all atoms)
Arg56	Glu41	-	-	Too Long		Too Long	
Ser57	Glu42	-	-	1.8337	2.1387	1.8194	2.1266
Gly58	Gly43	0.4093	0.4619	0.7992	0.8537	0.7834	0.8379
Val59	Ile44	-	-	0.4870	1.4130	0.4875	1.4151
Gly60	Gly45	0.5142	0.5109	0.4953	0.4869	0.4944	0.4876
Leu61	Leu46	0.4495	0.4802	0.4177	0.4842	0.4293	0.4902
Gln65	Gln50	0.1933	0.2696	0.4340	0.4239	0.4216	0.4156
Leu105	Ile86	-	-	0.9699	1.5517	0.9858	1.5510
Pro106	none	-	-	-	-	-	-
Thr107	none	-	-	-	-	-	-

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Gly108	Glu87	-	-	1.7757	1.7415	1.7446	1.7150
Glu109	Glu88	0.2880	0.3478	0.6969	0.5832	0.6699	0.5618
Gly110	Gly89	0.2008	0.1993	0.6020	0.4590	0.5843	0.4439
Cys111	Cys90	0.3367	0.4177	0.3111	0.4429	0.3104	0.4398
Leu112	Leu91	0.6834	0.9241	0.6170	0.8266	0.6151	0.8243
Asn117	Arg97	-	-	Too Long		Too Long	
Tyr147	Leu125	-	-	1.1351	1.1966	1.1011	1.1681
Ile150	Ile128	0.1519	0.3571	0.4175	0.5381	0.3877	0.5129
Val151	Cys129	-	-	0.5516	0.5981	0.5282	0.5765
His154	His132	0.2017	0.3312	0.2066	0.2882	0.2093	0.2909
Glu155	Glu133	0.2294	0.3944	0.3929	0.4743	0.3869	0.4745
His158	His136	0.2387	0.3944	0.2444	0.3116	0.2330	0.3050
Composite RMS		**0.36**	**0.46**	**0.83**	**0.98**	**0.81**	**0.97**

The active site of *S. aureus* pdf preferably includes at least a portion of the amino acids Gly58, Gly60, Leu61, Gln65, Glu109 , Gly110, Cys111, Leu112, Ile150, His154, Glu155, and His158; and more preferably at least a portion of the amino acids Arg56, Ser57, Gly58, Val59, Gly60, Leu61, Gln65, Leu105, Pro106, Thr107, Gly108, Glu109 , Gly110, Cys111, Leu112, Asn117, Tyr147, Ile150, Val151, His154, Glu155, and His158, as shown in Table 1. As used herein, "at least a portion of the amino acids" means at least about 50% of the amino acids, preferably at least about 70% of the amino acids, more preferably at least about 90% of the amino acids, and most preferably all the amino aicds. It will be readily apparent to those of skill in the art that the numbering of amino acids in other isoforms of *S. aureus* pdf may be different.

The amino acid constituents of an *S. aureus* pdf active site as defined herein, as well as selected constituent atoms thereof, are positioned in three dimensions in accordance with the structure coordinates listed in Table 1. In one aspect, the structure coordinates defining the active site of *S. aureus* pdf include structure coordinates of all atoms in the constituent amino acids; in another aspect, the structure coordinates of the active site include structure coordinates of just the backbone atoms of the constituent atoms.

The term "*S. aureus* pdf-like active site" refers to a portion of a molecule or molecular complex whose shape is sufficiently similar to at least a portion of the active site of *S. aureus* pdf as to be expected to bind related structural analogues. A structurally equivalent active site is defined by a root mean square deviation from the structure coordinates of the backbone atoms of the amino acids that make up the active sites in *S. aureus* pdf (as set forth in Table 1) of at most about 0.8 Å, and preferably less than about 0.35 Å. How this calculation is obtained is described below.

The term "associating with" refers to a condition of proximity between a chemical entity or compound, or portions thereof, and an *S. aureus* pdf molecule or portions thereof. The association may be non-covalent, wherein the juxtaposition is

energetically favored by hydrogen bonding, van der Waals forces, or electrostatic interactions, or it may be covalent.

Accordingly, the invention thus provides molecules or molecular complexes including an *S. aureus* pdf active site or *S. aureus* pdf-like active site, as defined by the sets of structure coordinates described above.

The crystal structure of the *Staphylococcus aureus* peptide deformylase enzyme (the def2 gene product) has been determined by MAD phased X-ray crystallography to 2.0 Å resolution. The protein structure reveals a fold similar to but not identical to the well characterized *E.coli* enzyme. Differences also extend into the active site region and will play a role in the elaboration of peptide deformylase (pdf) specific inhibitors.

Description of the Structure of pdf

The pdf structure is composed mostly of β-sheet with two lengthy helical regions near the n and c-terminus (Figure 5). The last helical region (147-161) forms the core of the structure and is also involved in catalysis. The β-sheet regions surround the centrally located, c-terminal helix and help to create the shallow cavity into which the substrates, formylated peptides, fit. The conserved motif HEXXH (H154 through H158) is found on this c-terminal helix and is involved in the coordination of the active site metal ion. Glutamic acid 155 is also likely essential for the catalytic process. Residues nearer the beginning of the helix are likely involved in specificity and are found near the opening of the cavity.

The n-terminal helical segments form a knot-like cluster on the "top" of the protein while the β-sheet regions are found on the lower half of the protein. A "thumb" region of coil extends from the lower sheet and covers the top of the metal ion (Center left Figure 6). The β-sheet rich section is composed of three β-sheet elements, an n-terminal anti-paralell three stranded β-sheet, a central anti-paralell three stranded β-sheet and a c-terminal mixed β-sheet. The β-sheet elements pack around the active site helix and form the walls of the active site cavity. The c-

terminus of the protein forms a last short strand of mixed β-sheet and is poised at the mouth of the active site (Figure 7).

The structure has a large number of well ordered waters which have been placed into the electron density maps based upon 3 sigma difference density during the refinement as well as the potential for good hydrogen bonding. Many waters fill the active site cavity.

The electrostatic surface potential of pdf indicates an intense positively charged surface at the back of the active site cavity—due to the presence of the metal ion. The upper surface of the protein is richly decorated with negatively charged residues, while the lower surface is generally more neutral in potential (Figure 8).

The active site metal ion.

A large body of experimental data including X-ray and NMR structures suggests that pdf contains a metal ion in the active site (Meinnel et al., *J. Bacteriol.*, 175:993-1000 (1993); Meinnel et al., *J. Bacteriol.*, 177:1883-87 (1995); Chan et al., *Biochemistry*, 36:13904-09 (1997)). In addition, activity data (Rajagopalan et al., *Biochemistry*, 36:13910-18 (1997); Rajagopalan et al., *J.Am.Chem.Soc.*, 119:12418-19 (1997)) point to iron as the most active metal ion. Data is consistent with this view; however, we have no experimental evidence based upon the present X-ray data to distinguish among ions like nickel, iron or zinc. From the initial MAD map it was clear that that a tetrahedrally coordinated metal ion is found in the three-dimensional structure of *S.aureus* pdf with water and the protein sidechains H154, H158, and C111 coordinating the metal ion. The sequence motif HEXXH (Mazel et al., *EMBO J.*, 13:914-23 (1994)) in the c-terminal helix is a signature motif which is found in many metalloproteases including thermolysin (Blundell, *Nat.Struct.Biol.*, 1:73-75 (1994); Jongeneel et al., *FEBS Lett.*, 242: 211-14 (1989); Makarova et al., *J. Mol. Biology*, 292:11-17 (1999)). The glutamic acid residue of this motif probably plays a dual role in metal coordination and catalysis. The water

molecule, which is a metal ligand, is tightly held in place by this glutamate residue in the present crystal structure. This residue likely plays a role in the protonation and deprotonation of reaction intermediates during the catalytic cycle in a manner similar to the role of

the conserved glutamate in thermolysin (Matthews, *Acc.Chem.Res.*, 21: 333-40 (1988); Chan et al., *Biochemistry*, 36:13904-09 (1997)).

Comparison of *S.aureus* pdf to *E.coli* structure

With the availability of numerous *E.coli* pdf X-ray and NMR structures (Table 1), it is possible to carry out a detailed comparison between these related enzymes. It should first be noted that the sequence identity between the *E.coli* and *S.aureus* enzymes is 45/134 or 33.5%. The rmsd for 134 α-carbons is 1.101 Å (1.457 Å for 861 common atoms; 1.189 Å for 536 main chain atoms). The vast majority of the identities (shown in Figure 10) are limited to the conserved motifs (metal binding regions). A structure-based alignment of the protein sequence is given in Figure 10. The poor sequence identity is not reflected in overall structural similarity. Both enzymes possess similar features in tertiary structure (Figure 11).

S.aureus pdf has seven insertions with respect to the *E.coli* sequence (Figure 10). The first insertion T3-M4 adds some additional hydrophobic surface area which forms a small surface for interaction with the third insertion (the extended n-terminal helix) N43-G54. The insertion after P25 adds one additional residue to the turn, which leads into the first long helix of pdf. This n-terminal helix is extended by an additional helix (insertion three N43-G54) which is not present in the *E.coli* structure. In the *E.coli* structure this helix is followed by a beta turn which drops down into the very conserved GXGLAA sequence which forms the third (and edge) strand of the n-terminal β-sheet. This strand also forms part of the wall of the active site crevice and provides loci for hydrogen bonding of peptide substrates (Hao et al., *Biochemistry*, 38: 4712-19 (1999)). The insertion of residues G81-G83 in the *S.aureus* structure extends the turn between strands II and III of the n-terminal β-

sheet. The insertion of V100 is in the turn between strand I of the central anti-parallel β-sheet and the central strand of the c-terminal mixed sheet. Insertion six occurs at the end of the central strand of the mix sheet and includes P106 and T107. These residues are positioned at the opening of the active site crevice and may be important determinates of *S.aureus* specificity. The subsequent conserved residues EGCLS form the other wall of the active site crevice. Residue C111 at the center of this sequence is one of the active site metal ligands. The conserved glutamic acid projects downward to form a part of the crevice wall and makes a conserved salt bridge with R124, which is found in the center of the first strand of the mix β-sheet. The insertion of A119 results in a slight bulge of the connecting strand (with respect to the *E.coli* structure) which precedes the first strand of the c-terminal mixed β-sheet. This seventh insertion, the sixth insertion (P106/T107) [both located in the thumb] and the c-terminal extension are all in close proximity and constitute a *S.aureus* specific surface.

From the simplest comparison of these two X-ray structures one is immediately struck by the obvious difference at the c-terminus (Figure 11). The *E.coli* enzyme has a long protruding α-helix which abutts the protein surface behind the active site cavity. The c-terminus of the *S.aureus* enzyme does not contain an equivalent α-helix, but wraps around the lower aspect of the thumb region to make a short stretch of β-sheet, terminating near the opening of the active site cavity. This is the major topological difference between the two structures, otherwise the proteins follow the same pattern and direction of secondary structure. Superposition of the two proteins permits a more detailed comparison of the alignment of secondary structural elements (Figure 12) and was the basis of the structure-based sequence alignment of Figure 10. A superficial evaluation would suggest that the core α-helix and the surrounding β-sheet is the most closely conserved region of the two proteins. Loops near the surface tend to be the location of insertions as is discussed above.

It follows from the low sequence identity between these two proteins, that the lining of the active site cavity would not be identical between *S.aureus* and *E.coli*. This expectation is in fact born out by the present structure (Figure 13). Analysis of the active site cavity suggests that 9 residue changes are found in the crevice and the annulus about the crevice. These changes are indicated in the table below (Table 4). Some particularly interesting changes include the replacement of R56 (*S.aureus*) for R97 (*E.coli*) where the arginine sidechain is conserved but changes the side of the cavity from which it projects. A number of subtle hydrophobic-hydrophobic changes are observed as are a number of polar-polar changes.

Table 4. Difference in the active site residue between *S.aureus* and *E.coli* pdf.

S.aureus	***E.coli***	***S.aureus***	***E.coli***
V59	I44	T107	E87
S57	E42	P106	----
R56	E41	L105	I86
N117	R97	Y147	L125
I150	I128	V151	C129

The X-ray structure of the (S)-2-O-(H-phosphonoxy)-L-caproyl-L-leucyl-p-nitroanilide (PCLNA) with the *E.coli* pdf enzyme (Hao et al., *Biochemistry*, 38: 4712-19 (1999)) can be used to guide the identification of the subsites (active sites) within the enzyme which accommodate the substrate amino acid sidechains (Schechter et al., *BBRC*, 27:157-62 (1967)). Using this scheme, the methionine analogue (caproyl), the P1 subsituent, would occupy the S1 subsite; leucine, P2, the S2 subsite; and the p-nitroanilide, P3, the S3 subsite. With the PCLNA inhibitor as a frame of reference, superposition (as above) with the present *S.aureus* pdf X-ray structure permits the general comparison of the *S.aureus* with the corresponding *E.coli* subsites. This comparison is schematically shown in Figure 14. The β-sheet

mainchain conformation of the inhibitor forces the inhibitor subsituents to adopt the typical down-up-down disposition observed for most peptidomimetic inhibitors. The P1 and P3 subsituents interact via the intra-molecular hydrophobic interface (between the caproyl and aromatic ring) to form a continuous surface which fills the S1 and S3 subsites. The P2 subsituent projects away from the protein surface toward solvent.

Comparison of the *E.coli* and *S.aureus* crystal structures indicates that six residues in the region of the active site are conserved. In fact, five are always conserved in pdf sequences (ETB, data not shown). The residues come from the three regions of greatest sequence identity; Gxglaa, EGCls, and IxxqHexdhl, where the capitization indicates a conserved residue in the active site crevice. The first glycine is the lone invariant amino acid on the right side of the cleft (Figure 15). The glutamic-glycine-cysteine triplet forms the invariant left side of the crevice. Finally, isoleucine and histidine are found at the bottom of the active site crevice (Figure 15). These conserved residues form a continuous invariant surface which extends from the methionine (caproyl) site (S1) and up the left wall of the crevice. The variable residues encircle the upper aspect of the crevice. The differences account for the subtle differences in crevice shape when the two enzymes are compared---and presumably will be important determinates for inhibitor specificity.

The S1 subsite has the greatest surface conservation between *E.coli* and *S.aureus*. This is due to the sequence conservation (outlined above) of the amino acids which form the bottom of the crevice---primarily H154, which also coordinates the metal ion, and I150. The long and fairly narrow hydrophobic subsite appears well-designed to cradle the preferred methionine residue. The rightside crevice wall is defined by V59(I, *E.coli*), Y147L, I150I, V151C, and L105I (Figure 17). The subsite is an exclusive hydrophobic surface in *E.coli*; whereas, the hydroxyl group of Y147 introduces a potential hydrogen bonding group in the upper aspect of the rightside of the equivalent *S. aureus* subsite. The presence of the

cysteine in the *E.coli* enyzme may contribute to the instability of the enzyme and may offer an advantage when working with *S.aureus* pdf.

The S2 subsite is quite different between the two enzymes (Figure 18). In *E.coli* R97 projects over the central leftside of the crevice and with E42 slightly narrows the entrance to the subsite. The principle hydrophobic interaction of the P2, leucyl, is with L91(L112, in *S.aureus*). This residue is always hydrophobic, but not strictly conserved among pdf from different bacteria. The subsite continues unobstructed across the protein surface and is completely accessible to bulk solvent. In *S.aureus* pdf the *E.coli* R97 is lost and replaced with R56, which projects from the leftside of the crevice. Also, on the leftside the *E.coli* E42 is replaced with S57. The sidechain hydroxyl project directly into the S2 subsite and may provide a handle for P2 specific inhibitors directed towards *S.aureus*. Finally, the S2 subsite in *S.aureus* is obstructed by R56 which projects across the subsite limiting its depth, and concomitantly providing additional hydrogen bonding determinates.

The S3 subsite is a broad somewhat flat hydrophobic surface in both enzymes (Figure 19). Aside from an aliphatic contribution from E109, which is conserved among all pdf enzymes, there are no strictly conserved amino acids in the S3 subsite. The insertion of P106 broadens the subsite in the *S.aureus* species. The introduction of T107 for glutamatic acid is important as is the amino acid Y147 (as noted above). In the former case, the polar group projects into the subsite in the *S.aureus* protein and is available for a unique hydrogen bond. In addition the aromatic Y147 and the possible hydrogen bond from the hydroxyl differentiate the rightside of the S3 subsite. These differences between *S.aureus* and *E.coli* create distinct features for the S3 subsite, which may be exploited for bacteria-specific pdf inhibitors.

Three-Dimensional Configurations

The structure coordinates generated for *S. aureus* pdf or the *S. aureus* pdf/ligand complex or one of its active sites shown in Table 1 define a unique

configuration of points in space. Those of skill in the art understand that a set of structure coordinates for protein or an protein/ligand complex, or a portion thereof, define a relative set of points that, in turn, define a configuration in three dimensions. A similar or identical configuration can be defined by an entirely different set of coordinates, provided the distances and angles between coordinates remain essentially the same. In addition, a scalable configuration of points can be defined by increasing or decreasing the distances between coordinates by a scalar factor while keeping the angles essentially the same.

The present invention thus includes the three-dimensional configuration of points derived from the structure coordinates of at least a portion of an *S. aureus* pdf molecule or molecular complex, as shown in Table 1, as well as structurally equivalent configurations, as described below. Preferably, the three-dimensional configuration includes points derived from structure coordinates representing the locations of a plurality of the amino acids defining the *S. aureus* pdf active site. In one embodiment, the three-dimensional configuration includes points derived from structure coordinates representing the locations the backbone atoms of a plurality of amino acids defining the *S. aureus* pdf active site, preferably Gly58, Gly60, Leu61, Gln65, Glu109 , Gly110, Cys111, Leu112, Ile150, His154, Glu155, and His158; and more preferably Arg56, Ser57, Gly58, Val59, Gly60, Leu61, Gln65, Leu105, Pro106, Thr107, Gly108, Glu109 , Gly110, Cys111, Leu112, Asn117, Tyr147, Ile150, Val151, His154, Glu155, and His158. In another embodiment, the three-dimensional configuration includes points derived from structure coordinates representing the locations of the side chain and the backbone atoms (other than hydrogens) of a plurality of the amino acids defining the *S. aureus* pdf active site, preferably Gly58, Gly60, Leu61, Gln65, Glu109 , Gly110, Cys111, Leu112, Ile150, His154, Glu155, and His158; and more preferably Arg56, Ser57, Gly58, Val59, Gly60, Leu61, Gln65, Leu105, Pro106, Thr107, Gly108, Glu109 , Gly110, Cys111, Leu112, Asn117, Tyr147, Ile150, Val151, His154, Glu155, and His158.

Likewise, the invention also includes the three-dimensional configuration of points derived from structure coordinates of molecules or molecular complexes that are structurally homologous to *S. aureus* pdf, as well as structurally equivalent configurations. Structurally homologous molecules or molecular complexes are defined below. Advantageously, structurally homologous molecules can be identified using the structure coordinates of *S. aureus* pdf (Table 1) according to a method of the invention.

The configurations of points in space derived from structure coordinates according to the invention can be visualized as, for example, a holographic image, a stereodiagram, a model or a computer-displayed image, and the invention thus includes such images, diagrams or models.

Structurally Equivalent Crystal Structures

Various computational analyses can be used to determine whether a molecule or the active site portion thereof is "structurally equivalent," defined in terms of its three-dimensional structure, to all or part of *S. aureus* pdf or its active sites. Such analyses may be carried out in current software applications, such as the Molecular Similarity application of QUANTA (Molecular Simulations Inc., San Diego, CA) version 4.1, and as described in the accompanying User's Guide.

The Molecular Similarity application permits comparisons between different structures, different conformations of the same structure, and different parts of the same structure. The procedure used in Molecular Similarity to compare structures is divided into four steps: (1) load the structures to be compared; (2) define the atom equivalences in these structures; (3) perform a fitting operation; and (4) analyze the results.

Each structure is identified by a name. One structure is identified as the target (i.e., the fixed structure); all remaining structures are working structures (i.e., moving structures). Since atom equivalency within QUANTA is defined by user input, for the purpose of this invention equivalent atoms are defined as protein

backbone atoms (N, Cα, C, and O) for all conserved residues between the two structures being compared. A conserved residue is defined as a residue that is structurally or functionally equivalent. Only rigid fitting operations are considered.

When a rigid fitting method is used, the working structure is translated and rotated to obtain an optimum fit with the target structure. The fitting operation uses an algorithm that computes the optimum translation and rotation to be applied to the moving structure, such that the root mean square difference of the fit over the specified pairs of equivalent atom is an absolute minimum. This number, given in angstroms, is reported by QUANTA.

For the purpose of this invention, any molecule or molecular complex or active site thereof, or any portion thereof, that has a root mean square deviation of conserved residue backbone atoms (N, Cα, C, O) of less than about 1.4 Å, when superimposed on the relevant backbone atoms described by the reference structure coordinates listed in Table 1, is considered “structurally equivalent” to the reference molecule. That is to say, the crystal structures of those portions of the two molecules are substantially identical, within acceptable error. Particularly preferred structurally equivalent molecules or molecular complexes are those that are defined by the entire set of structure coordinates in Table 1, ± a root mean square deviation from the conserved backbone atoms of those amino acids of not more than 1.4 Å. More preferably, the root mean square deviation is less than about 0.8 Å, and preferably less than about 0.35 Å.

The term "root mean square deviation" means the square root of the arithmetic mean of the squares of the deviations. It is a way to express the deviation or variation from a trend or object. For purposes of this invention, the "root mean square deviation" defines the variation in the backbone of a protein from the backbone of *S. aureus* pdf or an active site portion thereof, as defined by the structure coordinates of *S. aureus* pdf described herein.

Machine Readable Storage Media

Transformation of the structure coordinates for all or a portion of *S. aureus* pdf or the *S. aureus* pdf/ligand complex or one of its active sites, for structurally homologous molecules as defined below, or for the structural equivalents of any of these molecules or molecular complexes as defined above, into three-dimensional graphical representations of the molecule or complex can be conveniently achieved through the use of commercially-available software.

The invention thus further provides a machine-readable storage medium including a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, displays a graphical three-dimensional representation of any of the molecule or molecular complexes of this invention that have been described above. In a preferred embodiment, the machine-readable data storage medium includes a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, displays a graphical three-dimensional representation of a molecule or molecular complex including all or any parts of an *S. aureus* pdf active site or an *S. aureus* pdf-like active site, as defined above. In another preferred embodiment, the machine-readable data storage medium displays a graphical three-dimensional representation of a molecule or molecular complex defined by the structure coordinates of all of the amino acids in Table 1, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 0.8 Å.

In an alternative embodiment, the machine-readable data storage medium includes a data storage material encoded with a first set of machine readable data which includes the Fourier transform of the structure coordinates set forth in Table 1, and which, when using a machine programmed with instructions for using said data, can be combined with a second set of machine readable data including the x-ray diffraction pattern of a molecule or molecular complex to determine at least a

portion of the structure coordinates corresponding to the second set of machine readable data.

For example, a system for reading a data storage medium may include a computer including a central processing unit ("CPU"), a working memory which may be, e.g., RAM (random access memory) or "core" memory, mass storage memory (such as one or more disk drives or CD-ROM drives), one or more display devices (e.g., cathode-ray tube ("CRT") displays, light emitting diode ("LED") displays, liquid cyrstal displays ("LCDs"), electroluminescent displays, vacuum fluorescent displays, field emission displays ("FEDs"), plasma displays, projection panels, etc.), one or more user input devices (e.g., keyboards, microphones, mice, touch screens, etc.), one or more input lines, and one or more output lines, all of which are interconnected by a conventional bidirectional system bus. The system may be a stand-alone computer, or may be networked (e.g., through local area networks, wide area networks, intranets, extranets, or the internet) to other systems (e.g., computers, hosts, servers, etc.). The system may also include additional computer controlled devices such as consumer electronics and appliances.

Input hardware may be coupled to the computer by input lines and may be implemented in a variety of ways. Machine-readable data of this invention may be inputted via the use of a modem or modems connected by a telephone line or dedicated data line. Alternatively or additionally, the input hardware may include CD-ROM drives or disk drives. In conjunction with a display terminal, a keyboard may also be used as an input device.

Output hardware may be coupled to the computer by output lines and may similarly be implemented by conventional devices. By way of example, the output hardware may include a display device for displaying a graphical representation of an active site of this invention using a program such as QUANTA as described herein. Output hardware might also include a printer, so that hard copy output may be produced, or a disk drive, to store system output for later use.

In operation, a CPU coordinates the use of the various input and output devices, coordinates data accesses from mass storage devices, accesses to and from working memory, and determines the sequence of data processing steps. A number of programs may be used to process the machine-readable data of this invention. Such programs are discussed in reference to the computational methods of drug discovery as described herein. References to components of the hardware system are included as appropriate throughout the following description of the data storage medium.

Machine-readable storage devices useful in the present invention include, but are not limited to, magnetic devices, electrical devices, optical devices, and combinations thereof. Examples of such data storage devices include, but are not limited to, hard disk devices, CD devices, digital video disk devices, floppy disk devices, removable hard disk devices, magneto-optic disk devices, magnetic tape devices, flash memory devices, bubble memory devices, holographic storage devices, and any other mass storage peripheral device. It should be understood that these storage devices include necessary hardware (e.g., drives, controllers, power supplies, etc.) as well as any necessary media (e.g., disks, flash cards, etc.) to enable the storage of data..

Structurally Homologous Molecules, Molecular Complexes, And Crystal Structures

The structure coordinates set forth in Table 1 can be used to aid in obtaining structural information about another crystallized molecule or molecular complex. A "molecular complex" means a protein in covalent or non-covalent association with a chemical entity or compound. The method of the invention allows determination of at least a portion of the three-dimensional structure of molecules or molecular complexes which contain one or more structural features that are similar to structural features of *S. aureus* pdf. These molecules are referred to herein as "structurally homologous" to *S. aureus* pdf. Similar structural features can include, for example, regions of amino acid identity, conserved active site or

binding site motifs, and similarly arranged secondary structural elements (e.g., α helices and β sheets). Optionally, structural homology is determined by aligning the residues of the two amino acid sequences to optimize the number of identical amino acids along the lengths of their sequences; gaps in either or both sequences are permitted in making the alignment in order to optimize the number of identical amino acids, although the amino acids in each sequence must nonetheless remain in their proper order. Preferably, two amino acid sequences are compared using the Blastp program, version 2.0.9, of the BLAST 2 search algorithm, as described by Tatusova et al., *FEMS Microbiol Lett.,* 174:247-50 (1999), and available at http://www.ncbi.nlm.nih.gov/gorf/bl2.html. Preferably, the default values for all BLAST 2 search parameters are used, including matrix = BLOSUM62; open gap penalty = 11, extension gap penalty = 1, gap x_dropoff = 50, expect = 10, wordsize = 3, and filter on. In the comparison of two amino acid sequences using the BLAST search algorithm, structural similarity is referred to as "identity." Preferably, a structurally homologous molecule is a protein that has an amino acid sequence sharing at least 65% identity with the amino acid sequence of *S. aureus* pdf (SEQ ID NO: 1). More preferably, a protein that is structurally homologous to *S. aureus* pdf includes at least one contiguous stretch of at least 50 amino acids that shares at least 80% amino acid sequence identity with the analogous portion of *S. aureus* pdf. Methods for generating structural information about the structurally homologous molecule or molecular complex are well-known and include, for example, molecular replacement techniques.

Therefore, in another embodiment this invention provides a method of utilizing molecular replacement to obtain structural information about a molecule or molecular complex whose structure is unknown including the steps of:

(a) crystallizing the molecule or molecular complex of unknown structure;

(b) generating an x-ray diffraction pattern from said crystallized molecule or molecular complex; and

(c) applying at least a portion of the structure coordinates set forth in Table 1 to the x-ray diffraction pattern to generate a three-dimensional electron density map of the molecule or molecular complex whose structure is unknown.

By using molecular replacement, all or part of the structure coordinates of *S. aureus* pdf or the *S. aureus* pdf/ligand complex as provided by this invention (and set forth in Table 1) can be used to determine the structure of a crystallized molecule or molecular complex whose structure is unknown more quickly and efficiently than attempting to determine such information *ab initio*.

Molecular replacement provides an accurate estimation of the phases for an unknown structure. Phases are a factor in equations used to solve crystal structures that cannot be determined directly. Obtaining accurate values for the phases, by methods other than molecular replacement, is a time-consuming process that involves iterative cycles of approximations and refinements and greatly hinders the solution of crystal structures. However, when the crystal structure of a protein containing at least a structurally homologous portion has been solved, the phases from the known structure provide a satisfactory estimate of the phases for the unknown structure.

Thus, this method involves generating a preliminary model of a molecule or molecular complex whose structure coordinates are unknown, by orienting and positioning the relevant portion of *S. aureus* pdf or the *S. aureus* pdf/ligand complex according to Table 1 within the unit cell of the crystal of the unknown molecule or molecular complex so as best to account for the observed x-ray diffraction pattern of the crystal of the molecule or molecular complex whose structure is unknown. Phases can then be calculated from this model and combined with the observed x-ray diffraction pattern amplitudes to generate an electron density map of the structure whose coordinates are unknown. This, in turn, can be subjected to any well-known model building and structure refinement techniques to provide a final, accurate structure of the unknown crystallized molecule or molecular complex (E. Lattman, "Use of the Rotation and Translation Functions,"

in *Meth. Enzymol.*, 115:55-77 (1985); M.G. Rossman, ed., "The Molecular Replacement Method," *Int. Sci. Rev. Ser.*, No. 13, Gordon & Breach, New York (1972)).

Structural information about a portion of any crystallized molecule or molecular complex that is sufficiently structurally homologous to a portion of *S. aureus* pdf can be resolved by this method. In addition to a molecule that shares one or more structural features with *S. aureus* pdf as described above, a molecule that has similar bioactivity, such as the same catalytic activity, substrate specificity or ligand binding activity as *S. aureus* pdf, may also be sufficiently structurally homologous to *S. aureus* pdf to permit use of the structure coordinates of *S. aureus* pdf to solve its crystal structure.

In a preferred embodiment, the method of molecular replacement is utilized to obtain structural information about a molecule or molecular complex, wherein the molecule or molecular complex includes at least one *S. aureus* pdf subunit or homolog. A "subunit" of *S. aureus* pdf is an *S. aureus* pdf molecule that has been truncated at the N-terminus or the C-terminus, or both. In the context of the present invention, a "homolog" of *S. aureus* pdf is a protein that contains one or more amino acid substitutions, deletions, additions, or rearrangements with respect to the amino acid sequence of *S. aureus* pdf, but that, when folded into its native conformation, exhibits or is reasonably expected to exhibit at least a portion of the tertiary (three-dimensional) structure of *S. aureus* pdf. For example, structurally homologous molecules can contain deletions or additions of one or more contiguous or noncontiguous amino acids, such as a loop or a domain. Structurally homologous molecules also include "modified" *S. aureus* pdf molecules that have been chemically or enzymatically derivatized at one or more constituent amino acid, including side chain modifications, backbone modifications, and N- and C-terminal modifications including acetylation, hydroxylation, methylation, amidation, and the attachment of carbohydrate or lipid moieties, cofactors, and the like.

A heavy atom derivative of *S. aureus* pdf is also included as an *S. aureus* pdf homolog. The term "heavy atom derivative" refers to derivatives of *S. aureus* pdf produced by chemically modifying a crystal of *S. aureus* pdf. In practice, a crystal is soaked in a solution containing heavy metal atom salts, or organometallic compounds, e.g., lead chloride, gold thiomalate, thiomersal or uranyl acetate, which can diffuse through the crystal and bind to the surface of the protein. The location(s) of the bound heavy metal atom(s) can be determined by x-ray diffraction analysis of the soaked crystal. This information, in turn, is used to generate the phase information used to construct three-dimensional structure of the protein (T.L. Blundell and N.L. Johnson, *Protein Crystallography*, Academic Press (1976)).

Because *S. aureus* pdf can crystallize in more than one crystal form, the structure coordinates of *S. aureus* pdf as provided by this invention are particularly useful in solving the structure of other crystal forms of *S. aureus* pdf or *S. aureus* pdf complexes.

The structure coordinates of *S. aureus* pdf in Table 1 are also particularly useful to solve the structure of crystals of *S. aureus* pdf, *S. aureus* pdf mutants or *S. aureus* pdf homologs co-complexed with a variety of chemical entities. This approach enables the determination of the optimal sites for interaction between chemical entities, including candidate *S. aureus* pdf modifiers and *S. aureus* pdf. Potential sites for modification within the various binding site of the molecule can also be identified. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between *S. aureus* pdf and a chemical entity. For example, high resolution x-ray diffraction data collected from crystals exposed to different types of solvent allows the determination of where each type of solvent molecule resides. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for their potential modification of *S. aureus* pdf.

All of the complexes referred to above may be studied using well-known x-ray diffraction techniques and may be refined versus x-ray data to an R value of

about 0.20 or less using computer software, such as X-PLOR (Yale University, (1992), distributed by Molecular Simulations, Inc.; see, e.g., Blundell & Johnson, *supra*; *Meth. Enzymol.*, Vol. 114 & 115, H.W. Wyckoff et al., eds., Academic Press (1985)). This information may thus be used to optimize known modifiers of *S. aureus* pdf activity, and more importantly, to design new modifiers of *S. aureus* pdf activity.

The invention also includes the unique three-dimensional configuration defined by a set of points defined by the structure coordinates for a molecule or molecular complex structurally homologous to *S. aureus* pdf as determined using the method of the present invention, structurally equivalent configurations, and magnetic storage media including such set of structure coordinates.

Further, the invention includes structurally homologous molecules as identified using the method of the invention.

Homology Modeling

Using homology modeling, a computer model of an *S. aureus* pdf homolog can be built or refined without crystallizing the homolog. First, a preliminary model of the *S. aureus* pdf homolog is created by sequence alignment with *S. aureus* pdf, secondary structure prediction, the screening of structural libraries, or any combination of those techniques. Computational software may be used to carry out the sequence alignments and the secondary structure predictions. Structural incoherences, e.g., structural fragments around insertions and deletions, can be modeled by screening a structural library for peptides of the desired length and with a suitable conformation. For prediction of the side chain conformation, a side chain rotamer library may be employed. Where the *S. aureus* pdf homolog has been crystallized, the final homology model can be used to solve the crystal structure of the homolog by molecular replacement, as described above. Next, the preliminary model is subjected to energy minimization to yield an energy minimized model. The energy minimized model may contain regions where stereochemistry restraints

are violated, in which case such regions are remodeled to obtain a final homology model. The homology model is positioned according to the results of molecular replacement, and subjected to further refinement including molecular dynamics calculations.

Rational Drug Design

Computational techniques can be used to screen, identify, select and design chemical entities capable of associating with *S. aureus* pdf or structurally homologous molecules. Knowledge of the structure coordinates for *S. aureus* pdf permits the design and/or identification of synthetic compounds and/or other molecules which have a shape complementary to the conformation of the *S. aureus* pdf binding site. In particular, computational techniques can be used to identify or design chemical entities that are potential modifiers of *S. aureus* pdf activity, such as inhibitors, agonists and antagonists, that associate with an *S. aureus* pdf active site or an *S. aureus* pdf-like active site. Potential modifiers may bind to or interfere with all or a portion of the active site of *S. aureus* pdf, and can be competitive, non-competitive, or uncompetitive inhibitors; or interfere with dimerization by binding at the interface between the two monomers. Once identified and screened for biological activity, these inhibitors/agonists/antagonists may be used therapeutically or prophylactically to block *S. aureus* pdf activity and, thus, block bacterial growth. Structure-activity data for analogs of ligands that bind to or interfere with *S. aureus* pdf or *S. aureus* pdf-like active sites can also be obtained computationally.

The term "chemical entity," as used herein, refers to chemical compounds, complexes of two or more chemical compounds, and fragments of such compounds or complexes. Chemical entities that are determined to associate with *S. aureus* pdf are potential drug candidates. Data stored in a machine-readable storage medium that displays a graphical three-dimensional representation of the structure of *S. aureus* pdf or a structurally homologous molecule, as identified herein, or portions

thereof may thus be advantageously used for drug discovery. The structure coordinates of the chemical entity are used to generate a three-dimensional image that can be computationally fit to the three-dimensional image of *S. aureus* pdf or a structurally homologous molecule. The three-dimensional molecular structure encoded by the data in the data storage medium can then be computationally evaluated for its ability to associate with chemical entities. When the molecular structures encoded by the data is displayed in a graphical three-dimensional representation on a computer screen, the protein structure can also be visually inspected for potential association with chemical entities.

One embodiment of the method of drug design involves evaluating the potential association of a known chemical entity with *S. aureus* pdf or a structurally homologous molecule, particularly with an *S. aureus* pdf active site or *S. aureus* pdf-like active site. The method of drug design thus includes computationally evaluating the potential of a selected chemical entity to associate with any of the molecules or molecular complexes set forth above. This method includes the steps of: (a) employing computational means to perform a fitting operation between the selected chemical entity and a active site of the molecule or molecular complex; and (b) analyzing the results of said fitting operation to quantify the association between the chemical entity and the active site.

In another embodiment, the method of drug design involves computer-assisted design of chemical entities that associate with *S. aureus* pdf, its homologs, or portions thereof. Chemical entities can be designed in a step-wise fashion, one fragment at a time, or may be designed as a whole or "de novo."

To be a viable drug candidate, the chemical entity identified or designed according to the method must be capable of structurally associating with at least part of an *S. aureus* pdf or *S. aureus* pdf-like active sites, and must be able, sterically and energetically, to assume a conformation that allows it to associate with the *S. aureus* pdf or *S. aureus* pdf-like active site. Non-covalent molecular interactions important in this association include hydrogen bonding, van der Waals

interactions, hydrophobic interactions, and electrostatic interactions. Conformational considerations include the overall three-dimensional structure and orientation of the chemical entity in relation to the active site, and the spacing between various functional groups of an entity that directly interact with the *S. aureus* pdf-like active site or homologs thereof.

Optionally, the potential binding of a chemical entity to an *S. aureus* pdf or *S. aureus* pdf-like active site is analyzed using computer modeling techniques prior to the actual synthesis and testing of the chemical entity. If these computational experiments suggest insufficient interaction and association between it and the *S. aureus* pdf or *S. aureus* pdf-like active site, testing of the entity is obviated. However, if computer modeling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to or interfere with an *S. aureus* pdf or *S. aureus* pdf-like active site. Binding assays to determine if a compound actually binds to *S. aureus* pdf can also be performed and are well known in the art. Binding assays may employ kinetic or thermodynamic methodology using a wide variety of techniques including, but not limited to, microcalorimetry, circular dichroism, capillary zone electrophoresis, nuclear magnetic resonance spectroscopy, fluorescence spectroscopy, and combinations thereof.

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with an *S. aureus* pdf or *S. aureus* pdf-like active site. This process may begin by visual inspection of, for example, an *S. aureus* pdf or *S. aureus* pdf-like active site on the computer screen based on the *S. aureus* pdf structure coordinates in Table 1 or other coordinates which define a similar shape generated from the machine-readable storage medium. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within the active site. Docking may be accomplished using software such as QUANTA and SYBYL, followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical entities. Examples include GRID (P.J. Goodford, *J. Med. Chem.,* 28:849-57 (1985); available from Oxford University, Oxford, UK); MCSS (A. Miranker et al., *Proteins: Struct. Funct. Gen.,*11:29-34 (1991); available from Molecular Simulations, San Diego, CA); AUTODOCK (D.S. Goodsell et al., *Proteins: Struct. Funct. Genet.,* 8:195-202 (1990); available from Scripps Research Institute, La Jolla, CA); and DOCK (I.D. Kuntz et al., *J. Mol. Biol.,* 161:269-88 (1982); available from University of California, San Francisco, CA).

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or complex. Assembly may be preceded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of *S. aureus* pdf. This would be followed by manual model building using software such as QUANTA or SYBYL (Tripos Associates, St. Louis, MO).

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include, without limitation, CAVEAT (P.A. Bartlett et al., in *Molecular Recognition in Chemical and Biological Problems*, Special Publ., Royal Chem. Soc., 78:182-96 (1989); G. Lauri et al., *J. Comput. Aided Mol. Des.,* 8:51-66 (1994); available from the University of California, Berkeley, CA); 3D database systems such as ISIS (available from MDL Information Systems, San Leandro, CA; reviewed in Y.C. Martin, *J. Med. Chem.* 35:2145-54 (1992)); and HOOK (M.B. Eisen et al., *Proteins: Struc., Funct., Genet.,* 19:199-221 (1994); available from Molecular Simulations, San Diego, CA).

S. aureus pdf binding compounds may be designed "de novo" using either an empty binding site or optionally including some portion(s) of a known modifier(s). There are many de novo ligand design methods including, without limitation, LUDI (H.-J. Bohm, *J. Comp. Aid. Molec. Design.,* 6:61-78 (1992); available from Molecular Simulations Inc., San Diego, CA); LEGEND (Y. Nishibata et al., *Tetrahedron,* 47:8985 (1991); available from Molecular

Simulations Inc., San Diego, CA); LeapFrog (available from Tripos Associates, St. Louis, MO); and SPROUT (V. Gillet et al., *J. Comput. Aided Mol. Design,* 7:127-53 (1993); available from the University of Leeds, UK).

Once a compound has been designed or selected by the above methods, the efficiency with which that entity may bind to or interfere with an *S. aureus* pdf or *S. aureus* pdf-like active site may be tested and optimized by computational evaluation. For example, an effective *S. aureus* pdf or *S. aureus* pdf-like active site modifier must preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient *S. aureus* pdf or *S. aureus* pdf-like active site modifiers should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole; more preferably, not greater than 7 kcal/mole. *S. aureus* pdf or *S. aureus* pdf-like active site modifiers may interact with the active site in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free entity and the average energy of the conformations observed when the modifier binds to the protein.

An entity designed or selected as binding to or interfering with an *S. aureus* pdf or *S. aureus* pdf-like active site may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target enzyme and with the surrounding water molecules. Such non-complementary electrostatic interactions include repulsive charge-charge, dipole-dipole, and charge-dipole interactions.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interactions. Examples of programs designed for such uses include: Gaussian 94, revision C (M.J. Frisch, Gaussian, Inc., Pittsburgh, PA (1995)); AMBER, version 4.1 (P.A. Kollman, University of California at San Francisco, (1995)); QUANTA/CHARMM (Molecular Simulations, Inc., San Diego, CA (1995)); Insight II/Discover (Molecular

Simulations, Inc., San Diego, CA (1995)); DelPhi (Molecular Simulations, Inc., San Diego, CA (1995)); and AMSOL (Quantum Chemistry Program Exchange, Indiana University). These programs may be implemented, for instance, using a Silicon Graphics workstation such as an Indigo^2 with "IMPACT" graphics. Other hardware systems and software packages will be known to those skilled in the art.

Another approach encompassed by this invention is the computational screening of small molecule databases for chemical entities or compounds that can bind in whole, or in part, to a *S. aureus* pdf or *S. aureus* pdf-like active site. In this screening, the quality of fit of such entities to the binding site may be judged either by shape complementarity or by estimated interaction energy (E.C. Meng et al., *J. Comp. Chem.*, 13:505-24 (1992)).

This invention also enables the development of chemical entities that can isomerize to short-lived reaction intermediates in the chemical reaction of a substrate or other compound that binds to or with *S. aureus* pdf. Time-dependent analysis of structural changes in *S. aureus* pdf during its interaction with other molecules is carried out. The reaction intermediates of *S. aureus* pdf can also be deduced from the reaction product in co-complex with *S. aureus* pdf. Such information is useful to design improved analogs of known modifiers of *S. aureus* pdf activity or to design novel classes of modifiers based on the reaction intermediates of the *S. aureus* pdf and modifier co-complex. This provides a novel route for designing *S. aureus* pdf modifiers with both high specificity and stability.

Yet another approach to rational drug design involves probing the *S. aureus* pdf crystal of the invention with molecules including a variety of different functional groups to determine optimal sites for interaction between candidate *S. aureus* pdf modifiers and the protein. For example, high resolution x-ray diffraction data collected from crystals soaked in or co-crystallized with other molecules allows the determination of where each type of solvent molecule sticks. Molecules that bind tightly to those sites can then be further modified and

synthesized and tested for their hepes protease inhibitor activity (J. Travis, *Science*, 262:1374 (1993)).

In a related approach, iterative drug design is used to identify modifiers of *S. aureus* pdf activity. Iterative drug design is a method for optimizing associations between a protein and a compound by determining and evaluating the three-dimensional structures of successive sets of protein/compound complexes. In iterative drug design, crystals of a series of protein/compound complexes are obtained and then the three-dimensional structures of each complex is solved. Such an approach provides insight into the association between the proteins and compounds of each complex. This is accomplished by selecting compounds with inhibitory activity, obtaining crystals of this new protein/compound complex, solving the three dimensional structure of the complex, and comparing the associations between the new protein/compound complex and previously solved protein/compound complexes. By observing how changes in the compound affected the protein/compound associations, these associations may be optimized.

Pharmaceutical Compositions

Pharmaceutical compositions of this invention include a potential modifier of *S. aureus* pdf activity identified according to the invention, or a pharmaceutically acceptable salt thereof, and a pharmaceutically acceptable carrier, adjuvant, or vehicle. The term "pharmaceutically acceptable carrier" refers to a carrier(s) that is "acceptable" in the sense of being compatible with the other ingredients of a composition and not deleterious to the recipient thereof. Optionally, the pH of the formulation is adjusted with pharmaceutically acceptable acids, bases, or buffers to enhance the stability of the formulated compound or its delivery form.

Methods of making and using such pharmaceutical compositions are also included in the invention. The pharmaceutical compositions of the invention can be administered orally, parenterally, by inhalation spray, topically, rectally, nasally, buccally, vaginally, or via an implanted reservoir. Oral administration or

administration by injection is preferred. The term parenteral as used herein includes subcutaneous, intracutaneous, intravenous, intramuscular, intra-articular, intrasynovial, intrasternal, intrathecal, intralesional, and intracranial injection or infusion techniques.

Dosage levels of between about 0.01 and about 100 mg/kg body weight per day, preferably between about 0.5 and about 75 mg/kg body weight per day of the *S. aureus* pdf inhibitory compounds described herein are useful for the prevention and treatment of *S. aureus* pdf mediated disease. Typically, the pharmaceutical compositions of this invention will be administered from about 1 to about 5 times per day or alternatively, as a continuous infusion. Such administration can be used as a chronic or acute therapy. The amount of active ingredient that may be combined with the carrier materials to produce a single dosage form will vary depending upon the host treated and the particular mode of administration. A typical preparation will contain from about 5% to about 95% active compound (w/w). Preferably, such preparations contain from about 20% to about 80% active compound.

In order that this invention be more fully understood, the following examples are set forth. These examples are for the purpose of illustration only and are not to be construed as limiting the scope of the invention in any way.

EXAMPLES

Example 1: Analysis of the Structure of *S. aureus* pdf

Cloning and Expression

The plasmid containing the pdf insert was purified and used to transform a competent strain of *E. coli* JM109. This cDNA clone used for protein expression and purification (R127K H186Q, highlighted in Figure 3) contained two mutations. The second mutation is confirmed to be in the HIS6 tag (near the c-terminus) and has no effect on Km or Kcat. The gene encodes a total of 189 residues including a c-terminal hexahis tag.

The pdf protein was expressed using LB with ampicillin (100 mg/L) in both the seed and production media. LB was prepared using Bacto-tryptone (10g), Bacto yeast (5g), and NaCl (5g) added per L of deioninzed water. The pH of the media was adjusted to 7.5 before sterilization with KOH. The LB broth was auotclaved for 20 minutes in 100 ml volumes in 500 ml wide mouth fermentation flasks. Ampicillin was filter sterilized and added just before innoculation. The 100 ml seed stock fermentations were carried out in 500 ml wide mouth flasks and were innoculated from agar cultures and were incubated overnight at 37°C with agitation at 200 revolutions per minute (rpm). The seed fermentations were used to inoculate at 2% the 100 ml production fermentations which were also carried out in 500 ml wide mouth flasks. These fermentations were incubated with agitation at 200 rpm for slightly longer than 2 hours and were then induced (OD 660 nm reached 0.6). IPTG was added to a final concentration of 0.4mM. The induced fermentations were continued for an additional 3.5 hours until the OD reached 3.0. Multiple fermentations produced a final harvest of 4-6 liters for purification.

For expression of selenomethionyl-Pdf, M9 glucose was utilized in 100 ml volumes containing ampicillin, thiamin, and PAS trace metal solution at 100 mg, 5 mg and 0.3 ml per liter of deionized water, respectively. Multiple shake flasks were used to attain the desired fermentation volume. Since JM109 is not a methionine auxotroph, incorporation of selenomethionine was accomplished through down regulation of methionine biosynthesis just prior to induction (Van Duyne, Standaert, 1993). The culture was grown in 500 ml wide mouth fermentation flasks at 37°C with an agitation rate of 200 rpm until A600 reached ca. 0.5 unit. At this point, the following filter sterilized amino acids were added to achieve down-regulation. DL-selenomethione, L-lysine, L-threonine and L-phenylalanine were added to final concentrations of 120 micrograms/ml. L-leucine, L-isoleucine and L-valine were added to final concentrations of 60 micrograms/ml. After 15-20 minutes, protein expression was induced by the addition of filter sterilized IPTG added to a final concentration of 0.4 mM. Growth of the culture was continued as

described for an additional 3 hours when A600 reached ca. 2 units. Cells were then harvested by centrifugation and stored at -80°C.

Purification

Cell paste from a two liter *E.coli* fermentation expressing *S.aureus* pdf was lysed in 50 mM Tris-HCl pH=8.0 with lysozyme dissolved at 1mg/ml. The suspension sat on ice for 10 minutes and large strand DNA was broken by repeatedly shearing with a syringe and 19 gauge Needle. Cell extract was collected and centrifuged at 20500 rpm for 40-45 minutes at 5°C. Ni-NTA resin from Qiagen was equilibrated in lysis buffer (without lysozyme) and stirred into the cell extract. The suspension was poured into a column, washed expensively with lysis buffer and pdf was eluted with lysis buffer containing 200mM imidazole. This protein designated as pdf1 was used for the first crystallization efforts, but required further purification (Figure 4).

The eluate from the nickel column was concentrated by ultrafiltration with an Amicon stirred cell under nitrogen at room temperature. Two forms of pdf were resolved by anionic (Q fast flow, Pharmacia) exchange chromatography (without baseline resolution) as follows. A concentrated sample was injected onto a 1mL column equilibrated with 25mM Tris-HCl, pH=8.0. Proteins were resolved with a linear gradient of NaCl. The two forms of pdf were collected separately for further analysis. No differences in SDS-PAGE moblilty or purity were observed. The first fraction had optimal activity while the second fraction had much less specific activity. Protein eluted in the early fraction of the gradient was collected and further concentrated in a stirred cell to the desired volume. Further purified pdf is referred to as pdf2, and improved purification is verified by Isoelectric focussing. Pdf was either delivered for crystallization experiments at this time, or was mixed with 50% glycerol and stored at -20°C. Enzyme assays have demonstrated that pdf is stable for over one year when stored in 50% glycerol at -20°C.

Selenomethionine pdf was purified for crystallization efforts as described above with the inclusion of 5mM BME to reduce the chance of selenomethionine oxidation.

Protein Preparation

Protein was delivered immediately following concentration of peak material from the anion exchange column. The buffer contained 25mM Tris pH=8.0 and approximately 50mM NaCl. Protein was adjusted to 30 mg/ml and exchanged into buffer containing 25mM Tris pH=8.0. Later batches of protein were received at a protein concentration of 60mg/ml. This protein was diluted in half with water and frozen immediately in 50 microliter aliquots for later experiments.

Crystallization of S.aureus pdf

The first batch of pdf2 was received for crystallization. Crystallization experiments began with commercially available, random sparse matrix screens. Drops of 1μL protein and 1 μL well solutions were set up in hanging drop vapor diffusion experiments at room temperature. Crystals grew in one week from 4 separate well conditions 6,15,18 and 22 of Hampton Crystal Screen I (Jancarik et al., *J. Appl. Cryst.*, 24:409-11 (1991)). Follow-up grid screens were simultaneously set up to optimize each crystallization condition and are described below.

Hampton Research Crystal Screen I, #6

Hampton Screen I, condition 6 contains 30% PEG 4000, 0.2M $MgCl_2$ and 0.1M Tris pH=8.5. Original crystals grew as long thin needle clusters. Sitting drop vapor diffusion experiments were set up by mixing 2 microliters pdf + 2 microliters reservoir solution. Crystals were optimized through a series of grid screens varying both PEG 4000 and $MgCl_2$ concentrations. Results from these screens produced larger rod crystals.

Micro-seeding was utilized in an attempt to grow individual crystals. Seed stocks were made by breaking off a large rod crystal and crushing it in 10 microliters of matching well solution. Serial dilutions of seed stocks were made to 10^{-4}. Freshly mixed drops of protein and well solution containing 0.1M Tris pH=8.5, 0.075M $MgCl_2$ and varying amounts of PEG 4000 were seeded at setup with a cat whisker by successively streaking the whisker across one row. Single, chunky crystals grew within two weeks up to 0.35x0.35x0.7 micrometer. Large crystals often contained a channel down the middle of the crystal. Crystals were successfully stabilized and slowly transferred into a cryo-preservation solution containing 25% PEG 4000, 0.1M Tris pH=8.5, 0.1M $MgCl_2$ and 25% glycerol. Crystals were frozen in liquid nitrogen for cryogenic data collection.

Hampton Research Crystal Screen I, #15

Condition # 15 of Crystal Screen I was the second solution to produce crystals in the original screens. This solution contains 30% PEG 8000, 0.2M ammonium sulfate (A/S) and 0.1M Cacodylic acid pH=6.5. The original hit contained twinned crystalline rods that spread throughout the drop. The crystals were improved by varying both PEG 8000 and ammonium sulfate. Crystals improved significantly through micro-seeding. Crystals could be easily transferred to stabilization solution and slowly soaked into cryo-protective solution containing 22% PEG 8000, 0.2M ammonium sulfate, 0.1M cacodylic acid pH=6.5 and 25% glycerol for freezing.

Hampton Research Crystal Screen I, #18

A third solution to yield crystals was condition # 18 of Crystal Screen I. The solution is 20% PEG 8000, 0.1 m Na cacodylate pH=6.5 and 0.2M Mg acetate. Crystals grew as small rods that were very difficult to optimize. Seeding enabled the growth of a few large crystals, but crystals were very fragile. In many cases, crystals could not be stabilized without major crystal cracking. Despite these

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difficulties, a couple crystals were successfully soaked into cryo-solution containing 20% PEG 8000, 0.1 M NaCacodylate pH=6.5 and 0.2M MgAcetate and 25% glycerol and frozen for data collection.

Hampton Research Crystal Screen I, #22

Crystals also appeared in condition #22 which contains 30% PEG 4000, 0.1M Tris pH=8.5 and 0.2M sodium acetate. Crystals also grew as rod clusters and were optimized as described above for condition #6. Tweaking of the PEG 400 and Na acetate as well as micro-seeding produced large single rods grown from the bridge. Crystals were slowly soaked into cryo-solution of 0.3M Na acetate, 24% PEG 4000, 0.1M Tris pH=8.5 and 25% glycerol. Crystals diffracted well to 2.0Å.

Selenomethionine pdf

Se-methionine pdf was prepared and initial crystallization experiments were set up in each of the four conditions as described above. An additional 5mM BME was added to the reservoir solutions to reduce the chance of oxidation. Crystals from condition #6 were optimized through micro-seeding and produced sizable crystals. Crystals were prepared for low temperature data collection.

Data Collection, Space Group Determination

A crystal was grown from 28% PEG 8000, 0.1M cacodylic acid pH=6.5 and 0.1M ammonium sulfate and measured 0.1x0.1x0.5 micrometer. This crystal was the result of the follow up experiments from the Hampton I #15 hits. The crystal was frozen as described above for low temperature data collection. Data was collected on a single Hi Star at a detector distance of 18cm and a temperature of 100 °K. Frames of 300 seconds, 0.25° omega oscillation, and $2\theta=15$ were collected. Data was not processed because the crystal appeared obviously twinned.

Another crystal was grown from 16% PEG 8000, 0.1M Cacodylic Acid pH=6.5 and 0.4M Mg Acetate. This crystal was the result of the follow up

experiments from the Hampton I #18 hits. The crystal was frozen and data was collected on the APS 17-ID beamline. The crystal diffracted to around 1.9 Å and about 400 frames of 0.5 degree oscillation data were collected (Table 5). The space group is $C222_1$ with unit cell parameters of a=94.296 Å, b=120.85 Å, c=47.88 Å, and $\alpha = \beta = \gamma = 90°$. Data collection ended since we were at the end of the run and the crystal was recovered at APS and refrozen for additional data collection. Data collection was continued on this crystal. Data was collected on a single Hi Star at detector distance of 12 cm and 300 seconds per frame. The 2θ angle was set to 15° with an omega oscillation of 0.25°. Several water flow problems were encountered during data collection. This data was complete to around 2.7 Å (100% observed) with the I/sigma dropping below 2.0 for the higher resolution data. This data was not used for calculations. Molecular replacement was attempted using this data, but was unsuccessful.

A Se-methionine crystal was grown from 22.5% PEG 4000, 0.1M Tris pH=8.5 and 0.075M $MgCl_2$. This crystal was the result of the follow up experiments from the Hampton I #6 hits. Data was collected on a dual Hi Star at 12cm and 100°K. Each frame oscillated 0.25° omega for 200 seconds at 2θ=-25°. Data collection statistics are summarized in Table 6. The space group is $C222_1$ with unit cell parameters of a=94.469 Å, b=121.965 Å, c=47.58 Å, and $\alpha = \beta = \gamma = 90°$. This crystal diffracted to around 2.0 Å resolution. This data set was used for molecular replacement studies, but these also failed to produce a good solution. This data suggested that a good data set could be obtained from these Se-Methionine crystals at APS.

Preliminary co-crystallization experiments began in an attempt to obtain a pdf complex with several leads as determined from screens. A crystal was grown in the presence of 10% DMSO and 2mM of a potential inhibitor as well as the reservoir solution containing 20% PEG 4000, 0.1M Tris pH=8.5 and 0.1M $MgCl_2$. This crystal was the result of the follow up experiments from the Hampton I #6 hits. The crystal measured 0.28x0.28x0.98 micrometer and was frozen for low

temperature data collection. Data was collected on a dual Hi Star at 100°K. The detector distance was 12cm and $2\theta=30°$. Each frame of 0.25° omega oscillation was exposed for 200 seconds. The crystal diffracted to 1.9 Å and was of the $C222_1$ space group with unit cell parameters of a= 94.95 Å, b=122.08 Å, c=47.73 Å, and $\alpha=\beta=\gamma=90°$. Data statistics are summarized in Table 7. This data was used for refinement after the pdf structure was solved by MAD phasing, but a bound inhibitor was not observed.

Additional Se-methionine crystals were prepared for MAD data collection at APS. A crystal grew from 19% PEG 4000, 0.075M $MgCl_2$ and 0.1m Tris pH=8.5. . This crystal was the result of the follow up experiments from the Hampton I #6 hits. A total of 3 data sets were collected on the 17-ID beamline at APS. The crystal to detector distance was 15cm, $2\theta=0$ and each frame of 0.5° was exposed for 0.5 seconds. The ring current was 96.4mA. A low data set was collected at a low $\lambda=1.03321$, an edge data set was collected at the adsorption edge of λ=0.0.97939, and a peak data set was collected at $\lambda=0.97928$. Data collection statistics are summarized in Table 8. The space group is $C222_1$ with unit cell parameters of a= 94.113 Å, b=121.873 Å, c=47.579 Å, and $\alpha=\beta=\gamma=90°$.

TABLE 5: Data collection statistics.

Å	Obs	Theory	%	Redund	Rsym	Pairs	%	Rshell	%	2s
to 4.090	2042	2343	87.15	3.86	0.065	1863	79.51	0.065	85.08	2.9
to 3.247	4094	4584	89.31	3.99	0.067	3737	81.52	0.069	62.43	4.1
to 2.837	6182	6780	91.18	4.07	0.067	5683	83.82	0.067	42.23	5.8
to 2.578	8269	8975	92.13	4.11	0.069	7634	85.06	0.079	26.72	7.8
to 2.393	10326	11156	92.56	4.13	0.071	9571	85.79	0.093	21.02	11.4
to 2.252	12312	13339	92.30	4.08	0.074	11360	85.16	0.114	17.26	12.4
to 2.139	14308	15515	92.22	3.96	0.077	13141	84.70	0.126	14.22	15.7
to 2.046	16170	17685	91.43	3.82	0.079	14655	82.87	0.146	12.01	18.3
to 1.967	17759	19839	89.52	3.70	0.081	15709	79.18	0.195	8.90	22.9
to 1.899	19024	22028	86.36	3.60	0.083	16453	74.69	0.242	6.89	28.1

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TABLE 6: Data collection statistics for data with I/sigma greater than 2.

Resolution Å	Ref Possible	Ref Observed	observations	R-factor	I/sigma
3.76	3005	2791	21889	8.88	58.19
2.98	2871	2629	23125	9.73	43.57
2.61	2852	2453	18757	14.62	22.66
2.37	2843	2340	11384	11.83	13.50
2.20	2811	2148	9136	23.25	9.48
2.07	2809	1427	4412	15.93	6.45
	17191	13788	88703	10.29	28.55

TABLE 7: Data collection statistics for data with I/sigma greater than 2.

Resolution Å	Ref Possible	Ref Observed	observations	R-factor	I/sigma
3.61	3392	3160	21173	2.27	70.5
2.87	3259	3117	15625	3.99	37.7
2.51	3214	2881	8737	6.74	16.4
2.28	3201	2686	6898	9.37	10.8
2.11	3209	2520	5961	10.51	8.87
2.00	3176	1945	4074	11.24	6.90
	19451	16309	62468	3.70	27.7

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TABLE 8: Data collection statistics.

stats low

Coverage Statistics ......Shell

Angstrms		#Obs	Theory	%Compl	Redund	Rsym	Pairs	%Pairs	Rshell	#Sigma	%<2s
to	4.091	2265	2343	96.67	4.46	0.028	2072	88.43	0.028	84.43	2.0
to	3.247	4503	4588	98.15	4.82	0.030	4249	92.61	0.032	64.10	2.4
to	2.837	6720	6792	98.94	5.10	0.033	6444	94.88	0.041	38.38	4.0
to	2.578	8925	8992	99.25	5.27	0.035	8646	96.15	0.048	26.64	5.6
to	2.393	11131	11185	99.52	5.35	0.037	10850	97.00	0.053	20.55	8.2
to	2.252	13312	13363	99.62	5.23	0.038	12969	97.05	0.056	17.44	10.4
to	2.139	15489	15533	99.72	5.07	0.039	14978	96.43	0.062	14.57	13.6
to	2.046	17604	17725	99.32	4.92	0.040	16869	95.17	0.067	12.58	15.0
to	1.967	19626	19868	98.78	4.74	0.041	18446	92.84	0.081	9.67	18.8
to	1.899	21519	22066	97.52	4.54	0.042	19661	89.10	0.107	7.97	22.2

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stats edge

Coverage Statistics ..... Shell

Angstrms		#Obs	Theory	%Compl	Redund	Rsym	Pairs	%Pairs	Rshell	#Sigma	%<2s
to	4.091	2249	2343	95.99	3.74	0.034	1577	67.31	0.034	81.38	2.1
to	3.247	4478	4588	97.60	4.17	0.037	3455	75.31	0.039	60.12	2.6
to	2.837	6688	6792	98.47	4.51	0.043	5468	80.51	0.061	33.75	5.2
to	2.578	8892	8992	98.89	4.76	0.048	7550	83.96	0.081	22.55	7.3
to	2.393	11088	11185	99.13	4.94	0.053	9682	86.56	0.095	16.88	10.6
to	2.252	13278	13363	99.36	5.03	0.057	11842	88.62	0.101	14.05	12.9
to	2.139	15478	15533	99.65	4.97	0.060	13963	89.89	0.107	11.68	17.4
to	2.046	17649	17725	99.57	4.86	0.062	15967	90.08	0.113	10.17	18.8
to	1.967	19761	19868	99.46	4.76	0.064	17876	89.97	0.129	7.54	24.6
to	1.899	21904	22066	99.27	4.62	0.065	19621	88.92	0.152	5.87	29.9

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stats peak

Coverage Statistics ...... Shell

Angstrms		#Obs	Theory	%Compl	Redund	Rsym	Pairs	%Pairs	Rshell	#Sigma	%<2s
to	4.091	2280	2343	97.31	3.60	0.038	1594	68.03	0.038	81.02	2.3
to	3.247	4480	4588	97.65	4.04	0.040	3446	75.11	0.041	59.39	3.0
to	2.837	6677	6792	98.31	4.41	0.046	5373	79.11	0.063	33.15	5.9
to	2.578	8881	8992	98.77	4.67	0.051	7393	82.22	0.081	22.29	7.5
to	2.393	11072	11185	98.99	4.87	0.056	9452	84.51	0.095	16.80	10.8
to	2.252	13247	13363	99.13	4.97	0.060	11527	86.26	0.105	13.87	13.5
to	2.139	15449	15533	99.46	4.92	0.063	13605	87.59	0.116	11.72	17.7
to	2.046	17637	17725	99.50	4.81	0.066	15657	88.33	0.123	10.11	19.0
to	1.967	19798	19868	99.65	4.70	0.069	17642	88.80	0.143	7.63	24.5
to	1.899	22008	22066	99.74	4.56	0.071	19528	88.50	0.168	6.04	29.2

Phase determination and Refinement

The structure of *S.aureus* pdf was determined by multiple anomalous dispersion (MAD) using synchrotron radiation. The MAD data set included data to 1.9 Å resolution. Anomalous difference Patterson maps revealed the expected six selenium sites for a single protein molecule in the asymmetric unit. An excellent well-phased map to 1.9 Å resolution was produced into which the protein model could be easily built. However, XPLOR refinement of this model did not result in a model with an R-factor below 30%. This was difficult to understand since the overall map quality was excellent and there was little remaining difference density unaccounted for. This refinement effort was eventually discontinued in favor of a second data set. The 2.0 Å resolution data from the pdf crystal was used for the refinement of the structure. These data did refine well and a final R-factor of 18.6% for this model with good geometry was obtained (Table 9).

The X-ray data for the MAD phasing of pdf was collected at the Advanced Photon Source and consisted of three separate wavelength experiments centered about the Selenium edge (low, 1.03321 Å; edge, 0.97939 Å; high, 0.97928 Å). Each of the data sets were indexed and integrated separately. The data sets were scaled together using the program SCALEIT in the CCP4 Program Suite (Collaborative Computational Project N4, *Acta Cryst.*, D50:760-63 (1994)). Patterson maps revealed six selenium sites whose locations were determined and refined by direct methods using SHELX (Sheldrick et al., *Acta Cryst.*, B51:423-31 (1995)). Heavy atom refinement and phase calculations were carried out using MLPHARE from CCP4 with all the data from 10 to 1.9 Å resolution. The resulting electron density map was readily interpreted and a model built. A density modified map was also calculated (MLPHARE), but the maps were not very different. Model building was done with the program CHAIN (Sack, *J.Mol.Graphics*, 6:224-25 (1988)) and LORE (Finzel, *Meth.Enzymol.*, 277:230-42 (1997)). Initial refinement was carried out with XPLOR (Brunger AT. X-PLOR version 3.1: Asystem for X-ray crystallography and NMR. New Haven: Yale Univ. Press, (1992)). However, the R-

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factor failed to fall below 30% after several cycles and with the inclusion of many waters. At that point the refinement of this data set was discontinued in favor of another data set.

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TABLE 9: Data collection and phasing statistics

	λ 1.03321 Å	λ 0.97939 Å	λ 0.97928 Å
Resolution	1.9 Å	1.9 Å	1.9 Å
Average redundancy	4.5	4.5	4.5
# unique reflections	21519	21904	22008
% completeness	97.5%	99.3%	99.7%
$R_{sym}^{\dagger}$	0.042	0.065	0.071
R_{sym} (1.96-1.89 shell)	0.107	0.152	0.168
R_{cullis} acentrics	1.70 (19034 refs)	0.87 (18878 refs)	0.57 (18899 refs)
R_{cullis} anomalous	0.98 (19178 refs)	0.64 (18418 refs)	0.58 (18679 refs)
Phasing Power			
Centrics	---	0.70	1.83
Acentrics	---	0.80	2.15
Mean FOM	overall	centric	acentric
Before solvent flattening	0.714 (21048ref)	0.627 (2014 refs)	0.724 (19034 refs)
After solvent flattening	0.788	---	---

Refinement of the data set.

This data was used for the further refinement of the native pdf structure. The partially refined model derived from the MAD map was rotated to an arbitrary initial position, stripped of water and cations, and used for molecular replacement (XPLOR). The rotation solutions were filtered with PC-refinement (Brunger, *Acta Crystallogr.*, A46:46-47 (1990)). The highest rotation function peak also resulted in the hghest PC-filtered peak (PC=0.194). The position of the rotated monomer was obtained by a translation search (again the highest peak in the map and 15.6 sigma above the mean). The solution obtained was consistent with the position of the molecule in the MAD map and had an initial R-factor of 39.6% for data from 20-2.5 Å resolution (9235 reflections). This structure was further refined with XPLOR positional refinement and waters and a Zinc atom incorporated into the model. The R-factor dropped to 21% with a Free-R-factor of just over 25%. A final cycle of refinement and rebuilding was employed using PROLSQ (Hendrickson et al., "Stereochemically restrained crystallographic least-squares refinement of macromolecule structures" in *Biomolecular Structure, Function and Evolution*, (R.Srinivasan, ed. 43-57) Pergamon Press, Oxford UK (1980)) which resulted in a final R-factor of 18.62% for 16266 reflections, 10-2.0 Å resolution data. The final agreement statistics (Table 10) and Ramachandran plot revealed a well-refined structure and are included below. Additional statistics were generated with PROCHECK (Laskowski et al., *J. Appl.Cryst.*, 26:283-91 (1993)). A comparison of the initial MAD map and the final refined map was produced in CHAIN.

TABLE 10: Final model agreement statistics for PDF data set.

Resolution:	**2.00 Angstrom**	
R-value:	**18.62% for 16,266 reflections (2sigma)**	
Atoms 1725 (305 waters); 1 Zinc		
Mean B-factor 15.0 Å^2		
Final Model rmsd from expected for restraint class:		
Distances:	**1-2 bonds**	**0.018 (0.030)**
	1-3 bond angle	**0.031 (0.040)**
	1-4 torsional	**0.029 (0.050)**
Planes	**peptides**	**0.016 (0.030)**
	Other	**0.014 (0.030)**
	chiral volumes	**0.204 (0.250)**
NonBonded	**1-4**	**0.174 (0.300)**
	H-bond	**0.204 (0.300)**
	other	**0.172 (0.300)**
Thermal	**1-2 mainchain**	**1.033 (1.500)**
	1-3	**1.676 (3.000)**
	1-2 sidechain	**2.109 (2.000)**
	1-3 sidechain	**3.293 (4.000)**

Comparison of S.aureus and E.coli pdf structures.

The final S.aureus pdf and the E.coli pdf complex with (S)-2-O-(H-phosphonoxy)-L-caproyl-L-leucyl-p-nitroanilide (PCLNA) (Hao et al., *Biochemistry*, 38: 4712-19 (1999)) were compared using SUPERPDB (Finzel, unpublished). Figures 6 and 11 were produced with MOLSCRIPT (Kraulis, *J. Appl. Cryst.*, 24:946-50 (1991)) and Raster 3D (Merritt et al., *Acta Cryst.*, D50:869-73 (1994)). Figures 8, 9, 12 and 13 were prepared with MOSAIC2. Figures 7 and 14 were prepared with CHAIN using PLOT.

The complete disclosure of all patents, patent applications including provisional applications, and publications, and electronically available material (e.g., GenBank amino acid and nucleotide sequence submissions) cited herein are incorporated by reference. The foregoing detailed description and examples have been given for clarity of understanding only. No unnecessary limitations are to be

understood therefrom. The invention is not limited to the exact details shown and described; many variations will be apparent to one skilled in the art and are intended to be included within the invention defined by the claims.

SEQUENCE LISTING FREE TEXT

SEQ ID NO:1 *Staphylococcus aureus* peptide deformylase with C-terminal 6xHis tag

SEQ ID NO:2 *Escherichia coli* peptide deformylase

SEQ ID NO:3 *Haemophilis influenzae* peptide deformylase

SEQ ID NO:4 *Bacillus subtilis* peptide deformylase

SEQ ID NO:5 *Mycoplasma pneumoniae* peptide deformylase

SEQ ID NO:6 *Staphylococcus aureus* def1 gene (Pseudo pdf)

TABLE 1: Structure Coordinates for *S. aureus* pdf

CRYST1	94.950	122.080	47.730	90.00	90.00	90.00			
SCALE1	0.010532	0.000000	0.000000	0.00000					
SCALE2	0.000000	0.008191	0.000000	0.00000					
SCALE3	0.000000	0.000000	0.020951	0.00000					
ATOM	1	N	MET	1	34.916	34.289	28.962	1.00	19.94
ATOM	2	CA	MET	1	34.532	33.707	30.269	1.00	17.68
ATOM	3	CB	MET	1	34.906	34.864	31.043	1.00	22.02
ATOM	4	CG	MET	1	34.249	35.660	31.315	1.00	26.50
ATOM	5	SD	MET	1	34.946	36.841	32.629	1.00	21.74
ATOM	6	CE	MET	1	34.539	36.320	34.127	1.00	24.64
ATOM	7	C	MET	1	33.437	33.258	30.418	1.00	14.02
ATOM	8	O	MET	1	32.276	33.920	29.938	1.00	26.24
ATOM	9	N	LEU	2	32.981	31.938	30.879	1.00	7.75
ATOM	10	CA	LEU	2	31.816	31.467	31.565	1.00	8.41
ATOM	11	CB	LEU	2	32.031	30.005	32.023	1.00	8.48
ATOM	12	CG	LEU	2	32.268	28.961	30.866	1.00	7.73
ATOM	13	CD1	LEU	2	32.614	27.626	31.509	1.00	9.08
ATOM	14	CD2	LEU	2	30.932	28.747	30.133	1.00	8.57
ATOM	15	C	LEU	2	31.402	32.379	32.708	1.00	9.38
ATOM	16	O	LEU	2	32.278	32.943	33.415	1.00	10.57
ATOM	17	N	THR	3	30.099	32.656	32.839	1.00	9.70
ATOM	18	CA	THR	3	29.624	33.466	33.943	1.00	10.89
ATOM	19	CB	THR	3	29.238	34.900	33.661	1.00	10.34
ATOM	20	OG1	THR	3	28.067	34.943	32.811	1.00	13.27
ATOM	21	CG2	THR	3	30.363	35.684	33.051	1.00	9.36
ATOM	22	C	THR	3	28.428	32.714	34.511	1.00	12.61
ATOM	23	O	THR	3	28.150	31.586	34.034	1.00	12.67
ATOM	24	N	MET	4	27.740	33.297	35.478	1.00	13.52
ATOM	25	CA	MET	4	26.570	32.603	36.027	1.00	12.96
ATOM	26	CB	MET	4	26.007	33.362	37.225	1.00	12.16
ATOM	27	CG	MET	4	26.954	33.492	38.401	1.00	12.58
ATOM	28	SD	MET	4	27.512	31.883	38.995	1.00	12.58
ATOM	29	CE	MET	4	25.972	31.153	39.545	1.00	11.19
ATOM	30	C	MET	4	25.497	32.343	34.975	1.00	13.01
ATOM	31	O	MET	4	24.627	31.474	35.142	1.00	11.54
ATOM	32	N	LYS	5	25.475	33.147	33.917	1.00	13.68
ATOM	33	CA	LYS	5	24.490	32.976	32.902	1.00	14.22
ATOM	34	CB	LYS	5	24.163	34.124	31.992	1.00	16.93
ATOM	35	CG	LYS	5	25.243	34.788	31.252	1.00	18.60
ATOM	36	CD	LYS	5	24.807	35.647	30.112	1.00	19.21

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	37	CE	LYS	5	23.755	36.633	30.201	1.00	17.56
ATOM	38	NZ	LYS	5	23.653	37.497	28.989	1.00	17.28
ATOM	39	C	LYS	5	24.684	31.690	32.119	1.00	13.07
ATOM	40	O	LYS	5	23.720	31.241	31.521	1.00	12.87
ATOM	41	N	ASP	6	25.880	31.127	32.131	1.00	12.68
ATOM	42	CA	ASP	6	26.110	29.855	31.443	1.00	10.98
ATOM	43	CB	ASP	6	27.608	29.644	31.134	1.00	11.64
ATOM	44	CG	ASP	6	28.053	30.725	30.147	1.00	12.48
ATOM	45	OD1	ASP	6	27.837	30.487	28.933	1.00	13.27
ATOM	46	OD2	ASP	6	28.505	31.815	30.591	1.00	11.62
ATOM	47	C	ASP	6	25.640	28.730	32.353	1.00	11.50
ATOM	48	O	ASP	6	25.445	27.605	31.881	1.00	11.74
ATOM	49	N	ILE	7	25.501	29.000	33.628	1.00	11.13
ATOM	50	CA	ILE	7	25.098	27.943	34.547	1.00	11.49
ATOM	51	CB	ILE	7	25.811	28.121	35.898	1.00	11.70
ATOM	52	CG1	ILE	7	27.331	27.997	35.581	1.00	11.93
ATOM	53	CD1	ILE	7	28.288	28.140	36.663	1.00	12.02
ATOM	54	CG2	ILE	7	25.417	27.057	36.887	1.00	11.40
ATOM	55	C	ILE	7	23.634	27.664	34.603	1.00	11.29
ATOM	56	O	ILE	7	22.817	28.487	34.999	1.00	12.63
ATOM	57	N	ILE	8	23.245	26.433	34.193	1.00	10.48
ATOM	58	CA	ILE	8	21.856	26.026	34.213	1.00	9.51
ATOM	59	CB	ILE	8	21.513	24.909	33.253	1.00	8.83
ATOM	60	CG1	ILE	8	22.221	23.575	33.487	1.00	7.90
ATOM	61	CD1	ILE	8	21.762	22.525	32.454	1.00	7.81
ATOM	62	CG2	ILE	8	21.684	25.377	31.803	1.00	9.89
ATOM	63	C	ILE	8	21.433	25.703	35.643	1.00	10.40
ATOM	64	O	ILE	8	22.205	25.174	36.456	1.00	9.94
ATOM	65	N	ARG	9	20.182	26.031	35.987	1.00	11.42
ATOM	66	CA	ARG	9	19.665	25.850	37.329	1.00	12.02
ATOM	67	CB	ARG	9	19.009	27.157	37.828	1.00	10.73
ATOM	68	CG	ARG	9	19.850	28.421	37.618	1.00	11.22
ATOM	69	CD	ARG	9	21.253	28.290	38.166	1.00	11.70
ATOM	70	NE	ARG	9	22.124	29.328	37.705	1.00	14.84
ATOM	71	CZ	ARG	9	22.235	30.599	38.010	1.00	15.66
ATOM	72	NH1	ARG	9	21.529	31.122	38.991	1.00	18.52
ATOM	73	NH2	ARG	9	22.902	31.393	37.188	1.00	14.81
ATOM	74	C	ARG	9	18.764	24.658	37.504	1.00	12.31
ATOM	75	O	ARG	9	18.267	24.036	36.555	1.00	14.42
ATOM	76	N	ASP	10	18.518	24.283	38.736	1.00	12.74

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TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	77	CA	ASP	10	17.674	23.150	39.113	1.00	13.72
ATOM	78	CB	ASP	10	17.681	22.953	40.600	1.00	14.31
ATOM	79	CG	ASP	10	16.924	21.758	41.104	1.00	14.46
ATOM	80	OD1	ASP	10	17.107	20.628	40.640	1.00	14.86
ATOM	81	OD2	ASP	10	16.146	21.966	42.029	1.00	16.72
ATOM	82	C	ASP	10	16.285	23.236	38.506	1.00	14.81
ATOM	83	O	ASP	10	15.531	24.212	38.663	1.00	15.66
ATOM	84	N	GLY	11	15.932	22.174	37.772	1.00	14.39
ATOM	85	CA	GLY	11	14.636	22.169	37.079	1.00	15.06
ATOM	86	C	GLY	11	14.962	22.038	35.578	1.00	15.47
ATOM	87	O	GLY	11	14.116	21.564	34.841	1.00	16.98
ATOM	88	N	HIS	12	16.200	22.335	35.197	1.00	16.07
ATOM	89	CA	HIS	12	16.564	22.199	33.771	1.00	15.33
ATOM	90	CB	HIS	12	17.798	22.984	33.422	1.00	14.11
ATOM	91	CG	HIS	12	18.137	23.113	31.958	1.00	12.04
ATOM	92	ND1	HIS	12	18.258	22.085	31.076	1.00	10.56
ATOM	93	CE1	HIS	12	18.600	22.523	29.883	1.00	9.61
ATOM	94	NE2	HIS	12	18.767	23.826	29.977	1.00	11.37
ATOM	95	CD2	HIS	12	18.457	24.243	31.262	1.00	11.65
ATOM	96	C	HIS	12	16.780	20.692	33.515	1.00	15.36
ATOM	97	O	HIS	12	17.443	19.998	34.299	1.00	14.84
ATOM	98	N	PRO	13	16.209	20.178	32.431	1.00	14.53
ATOM	99	CA	PRO	13	16.296	18.798	32.066	1.00	14.20
ATOM	100	CB	PRO	13	15.436	18.664	30.843	1.00	14.95
ATOM	101	CG	PRO	13	15.070	20.047	30.408	1.00	15.00
ATOM	102	CD	PRO	13	15.333	20.975	31.520	1.00	14.75
ATOM	103	C	PRO	13	17.704	18.221	31.869	1.00	13.44
ATOM	104	O	PRO	13	17.920	17.049	32.297	1.00	13.01
ATOM	105	N	THR	14	18.641	18.885	31.313	1.00	12.25
ATOM	106	CA	THR	14	20.006	18.412	31.110	1.00	12.11
ATOM	107	CB	THR	14	20.879	19.447	30.442	1.00	12.39
ATOM	108	OG1	THR	14	20.324	19.783	29.186	1.00	14.02
ATOM	109	CG2	THR	14	22.327	19.047	30.251	1.00	11.43
ATOM	110	C	THR	14	20.616	17.961	32.443	1.00	11.87
ATOM	111	O	THR	14	21.340	16.974	32.439	1.00	12.53
ATOM	112	N	LEU	15	20.236	18.589	33.544	1.00	11.35
ATOM	113	CA	LEU	15	20.691	18.204	34.862	1.00	10.88
ATOM	114	CB	LEU	15	20.289	19.242	35.945	1.00	9.29
ATOM	115	CG	LEU	15	20.941	20.618	35.797	1.00	10.23
ATOM	116	CD1	LEU	15	20.421	21.579	36.861	1.00	9.66

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	117	CD2	LEU	15	22.486	20.500	35.940	1.00	8.87
ATOM	118	C	LEU	15	20.276	16.823	35.350	1.00	10.52
ATOM	119	O	LEU	15	20.887	16.276	36.276	1.00	10.57
ATOM	120	N	ARG	16	19.281	16.212	34.728	1.00	12.62
ATOM	121	CA	ARG	16	18.760	14.908	35.102	1.00	12.70
ATOM	122	CB	ARG	16	17.252	15.021	35.435	1.00	11.19
ATOM	123	CG	ARG	16	16.965	15.901	36.689	1.00	12.05
ATOM	124	CD	ARG	16	17.589	15.300	37.922	1.00	12.29
ATOM	125	NE	ARG	16	17.174	15.869	39.202	1.00	14.07
ATOM	126	CZ	ARG	16	17.503	15.282	40.354	1.00	14.85
ATOM	127	NH1	ARG	16	18.257	14.175	40.357	1.00	13.47
ATOM	128	NH2	ARG	16	17.016	15.724	41.537	1.00	14.89
ATOM	129	C	ARG	16	19.050	13.808	34.098	1.00	13.29
ATOM	130	O	ARG	16	18.686	12.615	34.267	1.00	12.21
ATOM	131	N	GLN	17	19.716	14.156	33.007	1.00	14.43
ATOM	132	CA	GLN	17	20.112	13.203	31.993	1.00	14.49
ATOM	133	CB	GLN	17	20.423	13.917	30.676	1.00	15.50
ATOM	134	CG	GLN	17	19.172	14.623	30.150	1.00	19.61
ATOM	135	CD	GLN	17	19.464	15.367	28.883	1.00	22.76
ATOM	136	OE1	GLN	17	20.585	15.845	28.654	1.00	25.94
ATOM	137	NE2	GLN	17	18.516	15.484	27.983	1.00	25.81
ATOM	138	C	GLN	17	21.414	12.531	32.438	1.00	14.27
ATOM	139	O	GLN	17	22.117	12.968	33.350	1.00	13.89
ATOM	140	N	LYS	18	21.716	11.457	31.735	1.00	14.65
ATOM	141	CA	LYS	18	22.963	10.724	31.984	1.00	13.90
ATOM	142	CB	LYS	18	22.734	9.222	32.030	1.00	15.80
ATOM	143	CG	LYS	18	24.083	8.533	32.321	1.00	19.05
ATOM	144	CD	LYS	18	23.986	7.048	32.414	1.00	21.35
ATOM	145	CE	LYS	18	25.337	6.413	32.686	1.00	22.45
ATOM	146	NZ	LYS	18	25.078	4.922	32.839	1.00	26.17
ATOM	147	C	LYS	18	23.980	11.178	30.950	1.00	12.55
ATOM	148	O	LYS	18	23.801	10.968	29.753	1.00	14.36
ATOM	149	N	ALA	19	25.068	11.839	31.353	1.00	10.71
ATOM	150	CA	ALA	19	26.065	12.355	30.478	1.00	10.46
ATOM	151	CB	ALA	19	27.088	13.257	31.241	1.00	9.78
ATOM	152	C	ALA	19	26.749	11.295	29.636	1.00	11.00
ATOM	153	O	ALA	19	26.983	10.143	30.034	1.00	12.01
ATOM	154	N	ALA	20	27.080	11.667	28.404	1.00	10.99
ATOM	155	CA	ALA	20	27.720	10.828	27.437	1.00	9.79
ATOM	156	CB	ALA	20	27.497	11.492	26.021	1.00	8.56

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	157	C	ALA	20	29.232	10.755	27.581	1.00	9.39
ATOM	158	O	ALA	20	29.876	11.797	27.803	1.00	8.57
ATOM	159	N	GLU	21	29.758	9.569	27.411	1.00	9.74
ATOM	160	CA	GLU	21	31.202	9.379	27.439	1.00	11.72
ATOM	161	CB	GLU	21	31.512	7.905	27.257	1.00	17.23
ATOM	162	CG	GLU	21	31.202	6.871	28.231	1.00	22.07
ATOM	163	CD	GLU	21	32.063	6.663	29.432	1.00	26.07
ATOM	164	OE1	GLU	21	33.305	6.831	29.247	1.00	28.08
ATOM	165	OE2	GLU	21	31.599	6.155	30.497	1.00	27.56
ATOM	166	C	GLU	21	31.861	10.115	26.238	1.00	11.80
ATOM	167	O	GLU	21	31.417	10.185	25.089	1.00	11.59
ATOM	168	N	LEU	22	33.013	10.661	26.528	1.00	11.07
ATOM	169	CA	LEU	22	33.838	11.349	25.587	1.00	11.81
ATOM	170	CB	LEU	22	34.811	12.325	26.236	1.00	9.69
ATOM	171	CG	LEU	22	34.424	13.644	26.794	1.00	8.78
ATOM	172	CD1	LEU	22	34.103	14.677	25.719	1.00	8.17
ATOM	173	CD2	LEU	22	33.310	13.559	27.815	1.00	8.71
ATOM	174	C	LEU	22	34.675	10.321	24.815	1.00	13.30
ATOM	175	O	LEU	22	35.079	9.332	25.372	1.00	13.83
ATOM	176	N	GLU	23	34.852	10.597	23.535	1.00	16.09
ATOM	177	CA	GLU	23	35.751	9.770	22.737	1.00	17.85
ATOM	178	CB	GLU	23	35.257	9.636	21.289	1.00	23.31
ATOM	179	CG	GLU	23	33.952	8.895	21.273	1.00	29.61
ATOM	180	CD	GLU	23	33.367	8.488	19.961	1.00	34.86
ATOM	181	OE1	GLU	23	33.510	9.170	18.922	1.00	37.14
ATOM	182	OE2	GLU	23	32.683	7.419	19.974	1.00	37.69
ATOM	183	C	GLU	23	37.087	10.532	22.787	1.00	16.82
ATOM	184	O	GLU	23	37.021	11.729	22.817	1.00	16.18
ATOM	185	N	LEU	24	38.209	9.855	22.917	1.00	18.03
ATOM	186	CA	LEU	24	39.524	10.444	22.930	1.00	17.31
ATOM	187	CB	LEU	24	40.436	9.892	24.031	1.00	16.16
ATOM	188	CG	LEU	24	40.230	10.228	25.490	1.00	16.48
ATOM	189	CD1	LEU	24	40.257	11.765	25.662	1.00	17.54
ATOM	190	CD2	LEU	24	38.965	9.743	26.117	1.00	15.61
ATOM	191	C	LEU	24	40.173	10.220	21.558	1.00	17.41
ATOM	192	O	LEU	24	39.995	9.166	20.916	1.00	19.08
ATOM	193	N	PRO	25	40.912	11.204	21.075	1.00	15.93
ATOM	194	CA	PRO	25	41.141	12.448	21.731	1.00	14.52
ATOM	195	CB	PRO	25	42.287	13.063	20.900	1.00	14.29
ATOM	196	CG	PRO	25	42.036	12.531	19.526	1.00	15.30

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	197	CD	PRO	25	41.604	11.109	19.738	1.00	15.06
ATOM	198	C	PRO	25	39.995	13.443	21.653	1.00	13.35
ATOM	199	O	PRO	25	39.177	13.401	20.754	1.00	13.89
ATOM	200	N	LEU	26	39.985	14.367	22.602	1.00	13.79
ATOM	201	CA	LEU	26	38.996	15.418	22.666	1.00	12.59
ATOM	202	CB	LEU	26	39.082	16.256	23.904	1.00	12.08
ATOM	203	CG	LEU	26	38.886	15.669	25.289	1.00	12.93
ATOM	204	CD1	LEU	26	38.866	16.788	26.340	1.00	10.60
ATOM	205	CD2	LEU	26	37.642	14.803	25.381	1.00	12.07
ATOM	206	C	LEU	26	39.100	16.326	21.409	1.00	12.36
ATOM	207	O	LEU	26	40.197	16.480	20.886	1.00	12.03
ATOM	208	N	THR	27	37.963	16.834	20.967	1.00	12.65
ATOM	209	CA	THR	27	37.963	17.766	19.832	1.00	14.54
ATOM	210	CB	THR	27	36.532	18.035	19.308	1.00	15.30
ATOM	211	OG1	THR	27	35.727	18.682	20.310	1.00	15.81
ATOM	212	CG2	THR	27	35.847	16.719	18.948	1.00	14.42
ATOM	213	C	THR	27	38.493	19.093	20.391	1.00	15.69
ATOM	214	O	THR	27	38.511	19.249	21.642	1.00	15.10
ATOM	215	N	LYS	28	38.949	20.026	19.593	1.00	17.11
ATOM	216	CA	LYS	28	39.461	21.322	20.062	1.00	16.59
ATOM	217	CB	LYS	28	39.640	22.170	18.785	1.00	21.45
ATOM	218	CG	LYS	28	40.041	23.601	18.941	1.00	24.97
ATOM	219	CD	LYS	28	41.424	23.746	19.542	1.00	28.58
ATOM	220	CE	LYS	28	41.893	25.200	19.520	1.00	29.78
ATOM	221	NZ	LYS	28	43.362	25.231	19.863	1.00	30.20
ATOM	222	C	LYS	28	38.449	22.070	20.922	1.00	15.27
ATOM	223	O	LYS	28	38.795	22.754	21.899	1.00	14.45
ATOM	224	N	GLU	29	37.202	21.988	20.547	1.00	14.88
ATOM	225	CA	GLU	29	36.095	22.628	21.221	1.00	14.47
ATOM	226	CB	GLU	29	34.832	22.548	20.375	1.00	20.18
ATOM	227	CG	GLU	29	33.633	23.176	21.057	1.00	25.80
ATOM	228	CD	GLU	29	32.326	22.956	20.331	1.00	30.91
ATOM	229	OE1	GLU	29	32.201	21.989	19.520	1.00	32.53
ATOM	230	OE2	GLU	29	31.389	23.743	20.643	1.00	32.71
ATOM	231	C	GLU	29	35.873	22.024	22.595	1.00	13.31
ATOM	232	O	GLU	29	35.595	22.749	23.545	1.00	11.60
ATOM	233	N	GLU	30	35.940	20.686	22.711	1.00	12.75
ATOM	234	CA	GLU	30	35.795	20.032	24.009	1.00	10.36
ATOM	235	CB	GLU	30	35.700	18.517	23.814	1.00	10.77
ATOM	236	CG	GLU	30	34.365	18.110	23.139	1.00	12.50

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	237	CD	GLU	30	34.397	16.669	22.642	1.00	11.90
ATOM	238	OE1	GLU	30	35.467	16.104	22.370	1.00	12.79
ATOM	239	OE2	GLU	30	33.310	16.151	22.474	1.00	14.28
ATOM	240	C	GLU	30	36.936	20.426	24.950	1.00	9.86
ATOM	241	O	GLU	30	36.678	20.595	26.156	1.00	9.16
ATOM	242	N	LYS	31	38.154	20.617	24.466	1.00	9.50
ATOM	243	CA	LYS	31	39.272	21.016	25.315	1.00	10.37
ATOM	244	CB	LYS	31	40.624	20.903	24.615	1.00	10.65
ATOM	245	CG	LYS	31	40.935	19.492	24.109	1.00	10.14
ATOM	246	CD	LYS	31	42.376	19.413	23.639	1.00	12.65
ATOM	247	CE	LYS	31	42.773	18.053	23.142	1.00	13.40
ATOM	248	NZ	LYS	31	44.122	17.978	22.539	1.00	16.75
ATOM	249	C	LYS	31	39.056	22.437	25.839	1.00	11.34
ATOM	250	O	LYS	31	39.219	22.729	27.019	1.00	10.78
ATOM	251	N	GLU	32	38.652	23.343	24.963	1.00	12.34
ATOM	252	CA	GLU	32	38.358	24.725	25.267	1.00	13.73
ATOM	253	CB	GLU	32	37.914	25.458	23.995	1.00	18.88
ATOM	254	CG	GLU	32	38.998	25.596	22.948	1.00	25.82
ATOM	255	CD	GLU	32	38.508	26.242	21.661	1.00	31.02
ATOM	256	OE1	GLU	32	37.329	26.619	21.506	1.00	34.16
ATOM	257	OE2	GLU	32	39.333	26.362	20.729	1.00	33.69
ATOM	258	C	GLU	32	37.266	24.829	26.333	1.00	12.41
ATOM	259	O	GLU	32	37.312	25.639	27.241	1.00	11.77
ATOM	260	N	THR	33	36.250	23.978	26.208	1.00	12.31
ATOM	261	CA	THR	33	35.163	23.899	27.157	1.00	12.37
ATOM	262	CB	THR	33	34.104	22.861	26.725	1.00	13.11
ATOM	263	OG1	THR	33	33.517	23.349	25.513	1.00	15.23
ATOM	264	CG2	THR	33	33.023	22.657	27.752	1.00	11.29
ATOM	265	C	THR	33	35.681	23.524	28.559	1.00	11.41
ATOM	266	O	THR	33	35.365	24.208	29.497	1.00	10.34
ATOM	267	N	LEU	34	36.486	22.474	28.658	1.00	11.17
ATOM	268	CA	LEU	34	37.030	22.021	29.928	1.00	10.16
ATOM	269	CB	LEU	34	37.678	20.654	29.693	1.00	9.41
ATOM	270	CG	LEU	34	38.102	19.874	30.942	1.00	8.70
ATOM	271	CD1	LEU	34	36.909	19.607	31.858	1.00	5.18
ATOM	272	CD2	LEU	34	38.697	18.541	30.452	1.00	8.15
ATOM	273	C	LEU	34	37.960	23.036	30.557	1.00	10.05
ATOM	274	O	LEU	34	37.967	23.258	31.785	1.00	10.33
ATOM	275	N	ILE	35	38.761	23.700	29.745	1.00	9.38
ATOM	276	CA	ILE	35	39.669	24.770	30.298	1.00	9.27

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	277	CB	ILE	35	40.619	25.168	29.153	1.00	9.96
ATOM	278	CG1	ILE	35	41.392	23.960	28.683	1.00	11.21
ATOM	279	CD1	ILE	35	42.276	24.096	27.476	1.00	10.72
ATOM	280	CG2	ILE	35	41.467	26.360	29.493	1.00	10.81
ATOM	281	C	ILE	35	38.843	25.908	30.801	1.00	8.81
ATOM	282	O	ILE	35	39.131	26.555	31.836	1.00	9.47
ATOM	283	N	ALA	36	37.769	26.277	30.047	1.00	8.60
ATOM	284	CA	ALA	36	36.878	27.369	30.469	1.00	8.07
ATOM	285	CB	ALA	36	35.833	27.665	29.390	1.00	8.37
ATOM	286	C	ALA	36	36.161	27.045	31.767	1.00	8.14
ATOM	287	O	ALA	36	35.768	27.917	32.560	1.00	8.12
ATOM	288	N	MET	37	35.881	25.724	31.941	1.00	8.77
ATOM	289	CA	MET	37	35.248	25.210	33.136	1.00	9.24
ATOM	290	CB	MET	37	34.795	23.764	33.059	1.00	8.72
ATOM	291	CG	MET	37	33.559	23.483	32.224	1.00	6.71
ATOM	292	SD	MET	37	33.335	21.789	31.709	1.00	6.53
ATOM	293	CE	MET	37	33.342	20.932	33.251	1.00	4.67
ATOM	294	C	MET	37	36.195	25.410	34.333	1.00	9.17
ATOM	295	O	MET	37	35.692	25.892	35.376	1.00	8.49
ATOM	296	N	ARG	38	37.452	25.050	34.165	1.00	8.88
ATOM	297	CA	ARG	38	38.401	25.295	35.266	1.00	8.29
ATOM	298	CB	ARG	38	39.761	24.673	34.946	1.00	6.27
ATOM	299	CG	ARG	38	40.886	25.129	35.854	1.00	6.22
ATOM	300	CD	ARG	38	42.253	24.472	35.513	1.00	6.20
ATOM	301	NE	ARG	38	43.275	24.989	36.431	1.00	8.87
ATOM	302	CZ	ARG	38	43.890	26.160	36.395	1.00	10.20
ATOM	303	NH1	ARG	38	43.647	27.040	35.409	1.00	11.24
ATOM	304	NH2	ARG	38	44.784	26.493	37.315	1.00	11.77
ATOM	305	C	ARG	38	38.583	26.825	35.430	1.00	9.07
ATOM	306	O	ARG	38	38.763	27.261	36.567	1.00	9.36
ATOM	307	N	GLU	39	38.575	27.572	34.337	1.00	8.69
ATOM	308	CA	GLU	39	38.771	29.029	34.403	1.00	9.54
ATOM	309	CB	GLU	39	39.029	29.643	33.049	1.00	10.78
ATOM	310	CG	GLU	39	39.650	31.040	33.051	1.00	14.31
ATOM	311	CD	GLU	39	41.070	30.997	33.632	1.00	17.29
ATOM	312	OE1	GLU	39	41.712	29.936	33.706	1.00	17.09
ATOM	313	OE2	GLU	39	41.577	32.041	34.079	1.00	19.58
ATOM	314	C	GLU	39	37.629	29.691	35.178	1.00	8.74
ATOM	315	O	GLU	39	37.872	30.680	35.887	1.00	8.33
ATOM	316	N	PHE	40	36.424	29.202	35.067	1.00	8.68

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	317	CA	PHE	40	35.267	29.674	35.808	1.00	8.98
ATOM	318	CB	PHE	40	33.969	28.890	35.546	1.00	6.33
ATOM	319	CG	PHE	40	32.816	29.364	36.423	1.00	7.37
ATOM	320	CD1	PHE	40	32.004	30.431	36.041	1.00	6.34
ATOM	321	CE1	PHE	40	30.944	30.806	36.826	1.00	7.39
ATOM	322	CZ	PHE	40	30.729	30.221	38.073	1.00	8.75
ATOM	323	CE2	PHE	40	31.553	29.164	38.474	1.00	7.42
ATOM	324	CD2	PHE	40	32.570	28.749	37.650	1.00	5.86
ATOM	325	C	PHE	40	35.567	29.539	37.321	1.00	9.68
ATOM	326	O	PHE	40	35.299	30.458	38.106	1.00	8.96
ATOM	327	N	LEU	41	36.096	28.389	37.716	1.00	8.34
ATOM	328	CA	LEU	41	36.407	28.121	39.108	1.00	7.20
ATOM	329	CB	LEU	41	36.736	26.662	39.311	1.00	5.79
ATOM	330	CG	LEU	41	35.632	25.661	38.986	1.00	4.96
ATOM	331	CD1	LEU	41	36.180	24.230	39.076	1.00	4.68
ATOM	332	CD2	LEU	41	34.592	25.769	40.118	1.00	5.67
ATOM	333	C	LEU	41	37.487	29.057	39.633	1.00	6.55
ATOM	334	O	LEU	41	37.318	29.593	40.732	1.00	6.21
ATOM	335	N	VAL	42	38.543	29.226	38.866	1.00	6.90
ATOM	336	CA	VAL	42	39.620	30.141	39.229	1.00	8.11
ATOM	337	CB	VAL	42	40.640	30.109	38.086	1.00	11.15
ATOM	338	CG1	VAL	42	41.734	31.155	38.206	1.00	13.45
ATOM	339	CG2	VAL	42	41.304	28.748	37.976	1.00	11.23
ATOM	340	C	VAL	42	38.991	31.513	39.408	1.00	8.71
ATOM	341	O	VAL	42	39.122	32.126	40.489	1.00	10.31
ATOM	342	N	ASN	43	38.252	32.049	38.442	1.00	8.34
ATOM	343	CA	ASN	43	37.596	33.354	38.565	1.00	8.46
ATOM	344	CB	ASN	43	36.811	33.707	37.239	1.00	8.52
ATOM	345	CG	ASN	43	37.814	34.020	36.161	1.00	9.24
ATOM	346	OD1	ASN	43	38.937	34.339	36.546	1.00	10.81
ATOM	347	ND2	ASN	43	37.464	33.943	34.891	1.00	10.73
ATOM	348	C	ASN	43	36.632	33.504	39.695	1.00	9.08
ATOM	349	O	ASN	43	36.559	34.588	40.314	1.00	8.98
ATOM	350	N	SER	44	35.887	32.473	40.035	1.00	9.07
ATOM	351	CA	SER	44	34.906	32.506	41.091	1.00	10.54
ATOM	352	CB	SER	44	33.940	31.317	41.107	1.00	9.94
ATOM	353	OG	SER	44	34.463	30.152	41.665	1.00	10.32
ATOM	354	C	SER	44	35.612	32.595	42.463	1.00	11.84
ATOM	355	O	SER	44	35.022	33.048	43.445	1.00	13.02
ATOM	356	N	GLN	45	36.866	32.177	42.517	1.00	12.29

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	357	CA	GLN	45	37.648	32.199	43.727	1.00	12.76
ATOM	358	CB	GLN	45	38.552	30.951	43.870	1.00	13.51
ATOM	359	CG	GLN	45	37.711	29.688	44.112	1.00	12.21
ATOM	360	CD	GLN	45	38.518	28.436	44.161	1.00	13.51
ATOM	361	OE1	GLN	45	39.733	28.479	44.331	1.00	15.12
ATOM	362	NE2	GLN	45	37.819	27.301	43.898	1.00	11.45
ATOM	363	C	GLN	45	38.451	33.491	43.882	1.00	14.04
ATOM	364	O	GLN	45	38.996	33.746	44.942	1.00	14.63
ATOM	365	N	ASP	46	38.518	34.305	42.869	1.00	14.76
ATOM	366	CA	ASP	46	39.203	35.595	42.881	1.00	17.02
ATOM	367	CB	ASP	46	39.977	35.835	41.627	1.00	20.12
ATOM	368	CG	ASP	46	40.799	37.118	41.646	1.00	23.64
ATOM	369	OD1	ASP	46	40.229	38.095	42.163	1.00	23.90
ATOM	370	OD2	ASP	46	41.954	37.141	41.179	1.00	26.97
ATOM	371	C	ASP	46	38.159	36.639	43.278	1.00	16.96
ATOM	372	O	ASP	46	37.141	36.906	42.690	1.00	15.76
ATOM	373	N	GLU	47	38.383	37.201	44.471	1.00	18.61
ATOM	374	CA	GLU	47	37.524	38.172	45.105	1.00	20.77
ATOM	375	CB	GLU	47	38.318	38.747	46.281	1.00	26.35
ATOM	376	CG	GLU	47	37.601	39.794	47.124	1.00	31.95
ATOM	377	CD	GLU	47	38.607	40.361	48.151	1.00	35.24
ATOM	378	OE1	GLU	47	39.590	41.011	47.707	1.00	36.36
ATOM	379	OE2	GLU	47	38.401	40.085	49.347	1.00	37.08
ATOM	380	C	GLU	47	37.043	39.303	44.202	1.00	20.14
ATOM	381	O	GLU	47	35.844	39.612	44.172	1.00	19.26
ATOM	382	N	GLU	48	37.975	39.957	43.516	1.00	19.74
ATOM	383	CA	GLU	48	37.697	41.040	42.619	1.00	20.15
ATOM	384	CB	GLU	48	39.015	41.724	42.176	1.00	26.28
ATOM	385	CG	GLU	48	38.788	42.838	41.175	1.00	33.55
ATOM	386	CD	GLU	48	39.965	43.661	40.716	1.00	38.79
ATOM	387	OE1	GLU	48	41.131	43.498	41.173	1.00	40.40
ATOM	388	OE2	GLU	48	39.734	44.559	39.829	1.00	39.98
ATOM	389	C	GLU	48	36.940	40.613	41.365	1.00	17.56
ATOM	390	O	GLU	48	35.980	41.201	40.970	1.00	15.31
ATOM	391	N	ILE	49	37.483	39.560	40.714	1.00	17.33
ATOM	392	CA	ILE	49	36.899	39.040	39.494	1.00	15.12
ATOM	393	CB	ILE	49	37.765	38.038	38.757	1.00	16.13
ATOM	394	CG1	ILE	49	39.111	38.674	38.292	1.00	16.15
ATOM	395	CD1	ILE	49	40.129	37.587	37.857	1.00	13.47
ATOM	396	CG2	ILE	49	36.997	37.575	37.496	1.00	16.11

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	397	C	ILE	49	35.503	38.558	39.794	1.00	13.80
ATOM	398	O	ILE	49	34.619	38.936	39.034	1.00	14.67
ATOM	399	N	ALA	50	35.287	37.841	40.890	1.00	12.57
ATOM	400	CA	ALA	50	33.952	37.373	41.233	1.00	12.32
ATOM	401	CB	ALA	50	33.951	36.441	42.447	1.00	10.25
ATOM	402	C	ALA	50	33.017	38.526	41.500	1.00	12.90
ATOM	403	O	ALA	50	31.824	38.435	41.186	1.00	12.81
ATOM	404	N	LYS	51	33.530	39.604	42.123	1.00	14.84
ATOM	405	CA	LYS	51	32.621	40.724	42.364	1.00	17.61
ATOM	406	CB	LYS	51	33.059	41.746	43.393	1.00	23.09
ATOM	407	CG	LYS	51	33.488	41.245	44.742	1.00	29.47
ATOM	408	CD	LYS	51	32.742	40.030	45.276	1.00	35.11
ATOM	409	CE	LYS	51	31.236	40.116	45.393	1.00	38.34
ATOM	410	NZ	LYS	51	30.581	38.814	45.690	1.00	39.45
ATOM	411	C	LYS	51	32.262	41.424	41.035	1.00	16.20
ATOM	412	O	LYS	51	31.066	41.571	40.745	1.00	17.61
ATOM	413	N	ARG	52	33.240	41.788	40.263	1.00	15.36
ATOM	414	CA	ARG	52	33.029	42.487	38.995	1.00	15.36
ATOM	415	CB	ARG	52	34.299	42.597	38.210	1.00	15.92
ATOM	416	CG	ARG	52	34.190	43.493	36.961	1.00	20.56
ATOM	417	CD	ARG	52	35.484	43.366	36.171	1.00	25.75
ATOM	418	NE	ARG	52	36.584	43.664	37.113	1.00	30.94
ATOM	419	CZ	ARG	52	37.845	43.340	36.840	1.00	34.86
ATOM	420	NH1	ARG	52	38.178	42.759	35.680	1.00	36.86
ATOM	421	NH2	ARG	52	38.734	43.409	37.825	1.00	36.03
ATOM	422	C	ARG	52	32.016	41.733	38.124	1.00	15.87
ATOM	423	O	ARG	52	31.146	42.328	37.514	1.00	15.88
ATOM	424	N	TYR	53	32.184	40.394	38.051	1.00	15.45
ATOM	425	CA	TYR	53	31.314	39.566	37.273	1.00	14.70
ATOM	426	CB	TYR	53	32.073	38.518	36.434	1.00	15.59
ATOM	427	CG	TYR	53	32.954	39.236	35.446	1.00	16.81
ATOM	428	CD1	TYR	53	32.407	39.794	34.291	1.00	17.94
ATOM	429	CE1	TYR	53	33.218	40.509	33.416	1.00	19.07
ATOM	430	CZ	TYR	53	34.568	40.622	33.684	1.00	19.48
ATOM	431	OH	TYR	53	35.396	41.309	32.827	1.00	22.92
ATOM	432	CE2	TYR	53	35.110	40.078	34.818	1.00	19.01
ATOM	433	CD2	TYR	53	34.301	39.379	35.692	1.00	18.15
ATOM	434	C	TYR	53	30.181	38.907	37.974	1.00	14.36
ATOM	435	O	TYR	53	29.510	38.141	37.274	1.00	15.28
ATOM	436	N	GLY	54	29.926	39.126	39.252	1.00	14.71

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	437	CA	GLY	54	28.814	38.492	39.937	1.00	15.24
ATOM	438	C	GLY	54	28.886	36.981	39.985	1.00	16.54
ATOM	439	O	GLY	54	27.879	36.281	39.822	1.00	19.66
ATOM	440	N	LEU	55	30.071	36.433	40.235	1.00	15.81
ATOM	441	CA	LEU	55	30.300	35.000	40.253	1.00	14.58
ATOM	442	CB	LEU	55	31.684	34.640	39.689	1.00	10.75
ATOM	443	CG	LEU	55	32.128	35.125	38.328	1.00	8.84
ATOM	444	CD1	LEU	55	33.483	34.650	37.920	1.00	6.15
ATOM	445	CD2	LEU	55	31.095	34.816	37.227	1.00	8.13
ATOM	446	C	LEU	55	30.165	34.407	41.645	1.00	14.82
ATOM	447	O	LEU	55	30.668	34.952	42.634	1.00	15.45
ATOM	448	N	ARG	56	29.397	33.312	41.702	1.00	13.86
ATOM	449	CA	ARG	56	29.268	32.583	42.994	1.00	14.05
ATOM	450	CB	ARG	56	27.988	31.773	42.901	1.00	12.84
ATOM	451	CG	ARG	56	27.702	30.880	44.040	1.00	12.65
ATOM	452	CD	ARG	56	26.371	30.171	43.928	1.00	13.01
ATOM	453	NE	ARG	56	26.264	29.199	44.998	1.00	13.72
ATOM	454	CZ	ARG	56	25.247	28.411	45.241	1.00	12.53
ATOM	455	NH1	ARG	56	24.176	28.440	44.495	1.00	10.89
ATOM	456	NH2	ARG	56	25.422	27.610	46.289	1.00	14.43
ATOM	457	C	ARG	56	30.501	31.671	43.133	1.00	14.45
ATOM	458	O	ARG	56	30.849	30.913	42.200	1.00	14.08
ATOM	459	N	SER	57	31.222	31.754	44.225	1.00	13.89
ATOM	460	CA	SER	57	32.426	30.929	44.412	1.00	15.05
ATOM	461	CB	SER	57	33.023	31.247	45.792	1.00	15.54
ATOM	462	OG	SER	57	34.277	30.604	45.995	1.00	17.22
ATOM	463	C	SER	57	32.107	29.424	44.362	1.00	14.39
ATOM	464	O	SER	57	31.028	29.003	44.817	1.00	14.42
ATOM	465	N	GLY	58	32.997	28.630	43.816	1.00	13.20
ATOM	466	CA	GLY	58	32.724	27.157	43.793	1.00	10.96
ATOM	467	C	GLY	58	34.050	26.420	43.697	1.00	8.84
ATOM	468	O	GLY	58	35.027	27.045	43.316	1.00	9.13
ATOM	469	N	VAL	59	34.082	25.126	43.982	1.00	8.47
ATOM	470	CA	VAL	59	35.220	24.274	43.887	1.00	7.38
ATOM	471	CB	VAL	59	35.731	23.702	45.248	1.00	6.40
ATOM	472	CG1	VAL	59	36.137	24.837	46.154	1.00	2.67
ATOM	473	CG2	VAL	59	34.729	22.751	45.834	1.00	6.06
ATOM	474	C	VAL	59	35.111	23.138	42.895	1.00	6.56
ATOM	475	O	VAL	59	36.087	22.423	42.623	1.00	5.81
ATOM	476	N	GLY	60	33.901	22.917	42.339	1.00	5.18

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	477	CA	GLY	60	33.686	21.922	41.328	1.00	3.01
ATOM	478	C	GLY	60	32.684	22.363	40.281	1.00	4.83
ATOM	479	O	GLY	60	31.831	23.228	40.563	1.00	7.05
ATOM	480	N	LEU	61	32.723	21.833	39.071	1.00	4.97
ATOM	481	CA	LEU	61	31.800	22.185	38.012	1.00	5.34
ATOM	482	CB	LEU	61	32.356	23.451	37.250	1.00	4.23
ATOM	483	CG	LEU	61	31.400	24.019	36.212	1.00	4.22
ATOM	484	CD1	LEU	61	30.116	24.482	36.841	1.00	2.46
ATOM	485	CD2	LEU	61	32.030	25.178	35.413	1.00	4.72
ATOM	486	C	LEU	61	31.694	21.018	37.026	1.00	5.60
ATOM	487	O	LEU	61	32.750	20.517	36.638	1.00	6.42
ATOM	488	N	ALA	62	30.504	20.552	36.686	1.00	5.63
ATOM	489	CA	ALA	62	30.418	19.406	35.741	1.00	4.65
ATOM	490	CB	ALA	62	29.619	18.292	36.364	1.00	2.45
ATOM	491	C	ALA	62	29.793	19.935	34.451	1.00	5.95
ATOM	492	O	ALA	62	28.964	20.817	34.490	1.00	6.05
ATOM	493	N	ALA	63	30.228	19.393	33.287	1.00	6.80
ATOM	494	CA	ALA	63	29.749	19.839	31.985	1.00	6.73
ATOM	495	CB	ALA	63	30.529	19.136	30.903	1.00	4.62
ATOM	496	C	ALA	63	28.270	19.965	31.891	1.00	8.06
ATOM	497	O	ALA	63	27.704	20.987	31.462	1.00	7.93
ATOM	498	N	PRO	64	27.455	19.043	32.424	1.00	9.12
ATOM	499	CA	PRO	64	25.985	19.168	32.412	1.00	8.90
ATOM	500	CB	PRO	64	25.605	17.981	33.293	1.00	8.17
ATOM	501	CG	PRO	64	26.622	16.974	32.833	1.00	7.79
ATOM	502	CD	PRO	64	27.917	17.751	32.936	1.00	8.59
ATOM	503	C	PRO	64	25.470	20.474	32.967	1.00	10.82
ATOM	504	O	PRO	64	24.417	21.004	32.529	1.00	12.14
ATOM	505	N	GLN	65	26.166	21.045	33.961	1.00	9.00
ATOM	506	CA	GLN	65	25.887	22.265	34.602	1.00	9.54
ATOM	507	CB	GLN	65	26.745	22.513	35.855	1.00	7.85
ATOM	508	CG	GLN	65	26.491	21.503	36.986	1.00	7.50
ATOM	509	CD	GLN	65	27.298	21.965	38.217	1.00	7.64
ATOM	510	OE1	GLN	65	28.430	21.506	38.343	1.00	6.16
ATOM	511	NE2	GLN	65	26.694	22.855	39.036	1.00	5.03
ATOM	512	C	GLN	65	25.965	23.523	33.712	1.00	9.56
ATOM	513	O	GLN	65	25.400	24.560	34.092	1.00	9.71
ATOM	514	N	ILE	66	26.607	23.468	32.580	1.00	9.17
ATOM	515	CA	ILE	66	26.768	24.427	31.569	1.00	8.61
ATOM	516	CB	ILE	66	28.175	24.958	31.202	1.00	7.57

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	517	CG1	ILE	66	29.148	23.899	30.706	1.00	7.91
ATOM	518	CD1	ILE	66	30.433	24.581	30.125	1.00	7.44
ATOM	519	CG2	ILE	66	28.749	25.769	32.340	1.00	7.53
ATOM	520	C	ILE	66	26.068	23.881	30.298	1.00	9.39
ATOM	521	O	ILE	66	26.309	24.232	29.163	1.00	10.40
ATOM	522	N	ASN	67	25.126	22.986	30.510	1.00	10.49
ATOM	523	CA	ASN	67	24.266	22.369	29.557	1.00	11.57
ATOM	524	CB	ASN	67	23.399	23.500	28.929	1.00	12.56
ATOM	525	CG	ASN	67	22.171	22.934	28.230	1.00	12.16
ATOM	526	OD1	ASN	67	21.751	21.813	28.405	1.00	12.53
ATOM	527	ND2	ASN	67	21.492	23.785	27.485	1.00	14.18
ATOM	528	C	ASN	67	24.980	21.596	28.464	1.00	11.97
ATOM	529	O	ASN	67	24.610	21.590	27.263	1.00	12.28
ATOM	530	N	ILE	68	26.093	21.000	28.821	1.00	10.89
ATOM	531	CA	ILE	68	26.918	20.161	27.888	1.00	10.88
ATOM	532	CB	ILE	68	28.298	20.745	27.721	1.00	10.24
ATOM	533	CG1	ILE	68	28.286	22.078	26.953	1.00	9.48
ATOM	534	CD1	ILE	68	29.646	22.766	26.933	1.00	7.35
ATOM	535	CG2	ILE	68	29.224	19.745	26.992	1.00	9.60
ATOM	536	C	ILE	68	26.868	18.749	28.499	1.00	10.44
ATOM	537	O	ILE	68	27.477	18.497	29.537	1.00	9.24
ATOM	538	N	SER	69	26.091	17.859	27.888	1.00	10.07
ATOM	539	CA	SER	69	25.867	16.541	28.468	1.00	10.16
ATOM	540	CB	SER	69	24.475	16.071	28.036	1.00	8.68
ATOM	541	OG	SER	69	23.982	14.974	28.781	1.00	9.95
ATOM	542	C	SER	69	26.972	15.562	28.156	1.00	10.74
ATOM	543	O	SER	69	26.778	14.529	27.532	1.00	11.54
ATOM	544	N	LYS	70	28.184	15.911	28.570	1.00	10.10
ATOM	545	CA	LYS	70	29.409	15.153	28.370	1.00	9.96
ATOM	546	CB	LYS	70	30.368	15.890	27.428	1.00	10.10
ATOM	547	CG	LYS	70	29.624	16.156	26.075	1.00	13.10
ATOM	548	CD	LYS	70	30.666	16.689	25.078	1.00	15.02
ATOM	549	CE	LYS	70	30.002	16.829	23.705	1.00	15.43
ATOM	550	NZ	LYS	70	30.955	17.277	22.697	1.00	17.50
ATOM	551	C	LYS	70	30.082	14.848	29.722	1.00	9.28
ATOM	552	O	LYS	70	29.937	15.649	30.656	1.00	10.48
ATOM	553	N	ARG	71	30.789	13.750	29.827	1.00	7.46
ATOM	554	CA	ARG	71	31.383	13.295	31.076	1.00	7.42
ATOM	555	CB	ARG	71	31.426	11.762	31.151	1.00	5.24
ATOM	556	CG	ARG	71	30.124	11.043	30.888	1.00	4.69

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	557	CD	ARG	71	30.141	9.561	31.166	1.00	3.45
ATOM	558	NE	ARG	71	30.097	9.086	32.533	1.00	5.53
ATOM	559	CZ	ARG	71	29.004	9.030	33.279	1.00	6.30
ATOM	560	NH1	ARG	71	27.846	9.361	32.738	1.00	6.87
ATOM	561	NH2	ARG	71	28.983	8.718	34.567	1.00	9.93
ATOM	562	C	ARG	71	32.756	13.852	31.351	1.00	7.34
ATOM	563	O	ARG	71	33.782	13.219	31.176	1.00	7.04
ATOM	564	N	MET	72	32.764	15.142	31.733	1.00	8.16
ATOM	565	CA	MET	72	33.929	15.899	32.038	1.00	7.49
ATOM	566	CB	MET	72	34.226	16.975	30.968	1.00	11.49
ATOM	567	CG	MET	72	34.482	16.514	29.597	1.00	14.92
ATOM	568	SD	MET	72	34.929	17.771	28.426	1.00	14.46
ATOM	569	CE	MET	72	33.462	18.708	28.193	1.00	15.90
ATOM	570	C	MET	72	33.639	16.756	33.276	1.00	6.05
ATOM	571	O	MET	72	32.583	17.367	33.360	1.00	5.46
ATOM	572	N	ILE	73	34.610	16.921	34.129	1.00	5.83
ATOM	573	CA	ILE	73	34.470	17.767	35.294	1.00	4.01
ATOM	574	CB	ILE	73	34.134	16.939	36.559	1.00	4.50
ATOM	575	CG1	ILE	73	35.208	15.825	36.788	1.00	3.12
ATOM	576	CD1	ILE	73	35.070	15.150	38.142	1.00	3.42
ATOM	577	CG2	ILE	73	32.758	16.373	36.503	1.00	3.16
ATOM	578	C	ILE	73	35.728	18.596	35.564	1.00	4.80
ATOM	579	O	ILE	73	36.814	18.324	35.070	1.00	4.39
ATOM	580	N	ALA	74	35.570	19.655	36.382	1.00	4.79
ATOM	581	CA	ALA	74	36.744	20.441	36.785	1.00	5.15
ATOM	582	CB	ALA	74	36.868	21.730	36.054	1.00	5.71
ATOM	583	C	ALA	74	36.659	20.559	38.308	1.00	4.79
ATOM	584	O	ALA	74	35.592	20.723	38.844	1.00	4.28
ATOM	585	N	VAL	75	37.774	20.324	39.020	1.00	6.37
ATOM	586	CA	VAL	75	37.811	20.449	40.484	1.00	6.45
ATOM	587	CB	VAL	75	37.984	19.144	41.290	1.00	5.03
ATOM	588	CG1	VAL	75	38.075	19.427	42.796	1.00	2.00
ATOM	589	CG2	VAL	75	36.744	18.271	41.056	1.00	3.76
ATOM	590	C	VAL	75	38.918	21.416	40.854	1.00	7.44
ATOM	591	O	VAL	75	40.043	21.229	40.321	1.00	8.86
ATOM	592	N	LEU	76	38.635	22.413	41.703	1.00	6.88
ATOM	593	CA	LEU	76	39.681	23.368	42.027	1.00	7.77
ATOM	594	CB	LEU	76	39.537	24.660	41.205	1.00	7.33
ATOM	595	CG	LEU	76	40.640	25.705	41.437	1.00	4.71
ATOM	596	CD1	LEU	76	41.961	25.218	40.861	1.00	3.93

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	597	CD2	LEU	76	40.257	27.038	40.857	1.00	7.52
ATOM	598	C	LEU	76	39.614	23.683	43.527	1.00	8.83
ATOM	599	O	LEU	76	38.896	24.560	43.956	1.00	10.55
ATOM	600	N	ILE	77	40.247	22.867	44.342	1.00	8.82
ATOM	601	CA	ILE	77	40.215	23.024	45.796	1.00	11.03
ATOM	602	CB	ILE	77	40.001	21.637	46.472	1.00	10.29
ATOM	603	CG1	ILE	77	38.674	21.025	46.000	1.00	9.23
ATOM	604	CD1	ILE	77	38.561	19.534	46.388	1.00	7.45
ATOM	605	CG2	ILE	77	39.946	21.906	48.012	1.00	11.93
ATOM	606	C	ILE	77	41.570	23.599	46.247	1.00	11.22
ATOM	607	O	ILE	77	42.605	22.996	46.058	1.00	11.78
ATOM	608	N	PRO	78	41.549	24.801	46.769	1.00	12.81
ATOM	609	CA	PRO	78	42.755	25.478	47.215	1.00	13.82
ATOM	610	CB	PRO	78	42.281	26.881	47.476	1.00	13.82
ATOM	611	CG	PRO	78	40.832	26.828	47.688	1.00	13.52
ATOM	612	CD	PRO	78	40.323	25.600	47.015	1.00	13.68
ATOM	613	C	PRO	78	43.384	24.865	48.463	1.00	14.04
ATOM	614	O	PRO	78	42.729	24.162	49.225	1.00	13.74
ATOM	615	N	ASP	79	44.663	25.190	48.665	1.00	15.66
ATOM	616	CA	ASP	79	45.421	24.733	49.796	1.00	16.97
ATOM	617	CB	ASP	79	46.815	25.342	49.773	1.00	17.17
ATOM	618	CG	ASP	79	47.725	24.835	50.845	1.00	19.81
ATOM	619	OD1	ASP	79	47.281	24.237	51.833	1.00	21.59
ATOM	620	OD2	ASP	79	48.968	24.997	50.743	1.00	23.71
ATOM	621	C	ASP	79	44.730	25.095	51.103	1.00	19.47
ATOM	622	O	ASP	79	44.386	26.257	51.328	1.00	19.81
ATOM	623	N	ASP	80	44.523	24.114	51.958	1.00	21.56
ATOM	624	CA	ASP	80	43.899	24.283	53.240	1.00	24.85
ATOM	625	CB	ASP	80	43.294	22.944	53.706	1.00	27.72
ATOM	626	CG	ASP	80	44.345	21.869	53.833	1.00	30.53
ATOM	627	OD1	ASP	80	44.094	20.790	54.401	1.00	32.70
ATOM	628	OD2	ASP	80	45.490	22.015	53.347	1.00	30.54
ATOM	629	C	ASP	80	44.898	24.740	54.318	1.00	26.28
ATOM	630	O	ASP	80	44.491	25.228	55.374	1.00	27.81
ATOM	631	N	GLY	81	46.168	24.602	54.112	1.00	26.90
ATOM	632	CA	GLY	81	47.214	24.943	55.079	1.00	27.17
ATOM	633	C	GLY	81	48.062	23.658	55.240	1.00	27.82
ATOM	634	O	GLY	81	49.259	23.728	55.546	1.00	28.21
ATOM	635	N	SER	82	47.391	22.520	54.989	1.00	27.02
ATOM	636	CA	SER	82	48.108	21.246	55.049	1.00	26.04

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	637	CB	SER	82	47.248	20.019	54.796	1.00	25.15
ATOM	638	OG	SER	82	46.765	20.059	53.446	1.00	26.13
ATOM	639	C	SER	82	49.127	21.195	53.882	1.00	24.89
ATOM	640	O	SER	82	50.066	20.426	53.980	1.00	25.62
ATOM	641	N	GLY	83	48.917	22.012	52.872	1.00	23.48
ATOM	642	CA	GLY	83	49.841	21.974	51.719	1.00	21.77
ATOM	643	C	GLY	83	49.163	21.092	50.638	1.00	19.26
ATOM	644	O	GLY	83	49.801	20.902	49.631	1.00	20.21
ATOM	645	N	LYS	84	47.972	20.576	50.867	1.00	16.73
ATOM	646	CA	LYS	84	47.296	19.797	49.836	1.00	14.79
ATOM	647	CB	LYS	84	46.528	18.644	50.415	1.00	16.65
ATOM	648	CG	LYS	84	47.294	17.703	51.325	1.00	20.53
ATOM	649	CD	LYS	84	46.320	16.536	51.571	1.00	26.25
ATOM	650	CE	LYS	84	46.765	15.630	52.681	1.00	29.35
ATOM	651	NZ	LYS	84	46.698	16.382	53.997	1.00	31.51
ATOM	652	C	LYS	84	46.305	20.645	49.058	1.00	13.36
ATOM	653	O	LYS	84	45.482	21.354	49.657	1.00	13.57
ATOM	654	N	SER	85	46.334	20.575	47.727	1.00	12.20
ATOM	655	CA	SER	85	45.399	21.352	46.904	1.00	10.79
ATOM	656	CB	SER	85	45.910	22.713	46.473	1.00	10.03
ATOM	657	OG	SER	85	46.979	22.545	45.587	1.00	12.27
ATOM	658	C	SER	85	45.052	20.517	45.660	1.00	9.97
ATOM	659	O	SER	85	45.892	19.710	45.314	1.00	9.45
ATOM	660	N	TYR	86	43.855	20.667	45.136	1.00	8.93
ATOM	661	CA	TYR	86	43.370	19.823	44.040	1.00	8.91
ATOM	662	CB	TYR	86	42.190	18.985	44.568	1.00	9.61
ATOM	663	CG	TYR	86	42.612	18.127	45.766	1.00	11.87
ATOM	664	CD1	TYR	86	42.525	18.675	47.031	1.00	12.22
ATOM	665	CE1	TYR	86	42.968	17.980	48.146	1.00	14.09
ATOM	666	CZ	TYR	86	43.464	16.693	47.998	1.00	13.74
ATOM	667	OH	TYR	86	43.877	16.050	49.147	1.00	14.04
ATOM	668	CE2	TYR	86	43.587	16.139	46.747	1.00	13.17
ATOM	669	CD2	TYR	86	43.136	16.849	45.631	1.00	12.81
ATOM	670	C	TYR	86	42.937	20.636	42.843	1.00	8.39
ATOM	671	O	TYR	86	42.041	21.470	42.905	1.00	11.10
ATOM	672	N	ASP	87	43.597	20.487	41.740	1.00	7.58
ATOM	673	CA	ASP	87	43.388	21.198	40.491	1.00	7.93
ATOM	674	CB	ASP	87	44.561	22.172	40.249	1.00	7.54
ATOM	675	CG	ASP	87	44.336	23.088	39.060	1.00	9.36
ATOM	676	OD1	ASP	87	43.367	22.912	38.300	1.00	9.22

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	677	OD2	ASP	87	45.098	24.043	38.908	1.00	12.88
ATOM	678	C	ASP	87	43.369	20.124	39.392	1.00	6.63
ATOM	679	O	ASP	87	44.445	19.695	38.965	1.00	7.41
ATOM	680	N	TYR	88	42.204	19.657	39.046	1.00	7.18
ATOM	681	CA	TYR	88	42.058	18.612	38.048	1.00	7.88
ATOM	682	CB	TYR	88	41.775	17.252	38.727	1.00	8.03
ATOM	683	CG	TYR	88	42.918	16.706	39.528	1.00	7.31
ATOM	684	CD1	TYR	88	43.051	16.986	40.887	1.00	7.10
ATOM	685	CE1	TYR	88	44.093	16.455	41.622	1.00	5.16
ATOM	686	CZ	TYR	88	45.017	15.649	40.992	1.00	5.90
ATOM	687	OH	TYR	88	46.088	15.153	41.721	1.00	7.39
ATOM	688	CE2	TYR	88	44.955	15.404	39.643	1.00	6.03
ATOM	689	CD2	TYR	88	43.866	15.894	38.917	1.00	6.97
ATOM	690	C	TYR	88	40.939	18.810	37.051	1.00	8.22
ATOM	691	O	TYR	88	39.816	19.193	37.355	1.00	9.63
ATOM	692	N	MET	89	41.231	18.498	35.814	1.00	8.89
ATOM	693	CA	MET	89	40.233	18.533	34.736	1.00	8.17
ATOM	694	CB	MET	89	40.600	19.441	33.591	1.00	7.98
ATOM	695	CG	MET	89	40.522	20.918	33.852	1.00	8.05
ATOM	696	SD	MET	89	41.005	21.973	32.496	1.00	8.41
ATOM	697	CE	MET	89	42.746	21.671	32.340	1.00	7.64
ATOM	698	C	MET	89	40.203	17.038	34.319	1.00	5.98
ATOM	699	O	MET	89	41.212	16.525	33.797	1.00	6.63
ATOM	700	N	LEU	90	39.123	16.386	34.611	1.00	4.43
ATOM	701	CA	LEU	90	39.050	14.952	34.284	1.00	5.33
ATOM	702	CB	LEU	90	38.707	14.179	35.541	1.00	6.25
ATOM	703	CG	LEU	90	39.564	14.222	36.755	1.00	6.92
ATOM	704	CD1	LEU	90	39.034	13.233	37.827	1.00	4.71
ATOM	705	CD2	LEU	90	41.018	13.889	36.453	1.00	6.93
ATOM	706	C	LEU	90	38.027	14.648	33.196	1.00	4.75
ATOM	707	O	LEU	90	36.963	15.237	33.151	1.00	5.61
ATOM	708	N	VAL	91	38.354	13.719	32.348	1.00	4.98
ATOM	709	CA	VAL	91	37.487	13.246	31.253	1.00	4.58
ATOM	710	CB	VAL	91	38.323	13.299	29.938	1.00	4.51
ATOM	711	CG1	VAL	91	37.590	12.571	28.815	1.00	6.97
ATOM	712	CG2	VAL	91	38.589	14.718	29.522	1.00	2.32
ATOM	713	C	VAL	91	37.137	11.805	31.576	1.00	5.04
ATOM	714	O	VAL	91	38.003	11.030	31.991	1.00	5.81
ATOM	715	N	ASN	92	35.842	11.420	31.481	1.00	5.85
ATOM	716	CA	ASN	92	35.357	10.088	31.747	1.00	6.19

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	717	CB	ASN	92	35.743	9.111	30.644	1.00	7.29
ATOM	718	CG	ASN	92	35.308	9.457	29.252	1.00	7.92
ATOM	719	OD1	ASN	92	34.247	10.045	29.090	1.00	7.73
ATOM	720	ND2	ASN	92	36.092	9.017	28.271	1.00	10.17
ATOM	721	C	ASN	92	35.756	9.501	33.083	1.00	8.19
ATOM	722	O	ASN	92	36.265	8.363	33.177	1.00	9.98
ATOM	723	N	PRO	93	35.644	10.283	34.153	1.00	8.97
ATOM	724	CD	PRO	93	35.059	11.684	34.132	1.00	7.81
ATOM	725	CA	PRO	93	35.996	9.859	35.482	1.00	8.04
ATOM	726	CB	PRO	93	35.928	11.155	36.272	1.00	7.31
ATOM	727	CG	PRO	93	34.802	11.890	35.596	1.00	7.53
ATOM	728	C	PRO	93	35.074	8.770	35.997	1.00	9.49
ATOM	729	O	PRO	93	33.852	8.750	35.756	1.00	9.28
ATOM	730	N	LYS	94	35.690	7.828	36.740	1.00	9.93
ATOM	731	CA	LYS	94	34.921	6.724	37.302	1.00	9.81
ATOM	732	CB	LYS	94	34.975	5.537	36.280	1.00	13.20
ATOM	733	CG	LYS	94	33.920	4.483	36.579	1.00	18.63
ATOM	734	CD	LYS	94	34.020	3.251	35.668	1.00	23.45
ATOM	735	CE	LYS	94	32.846	2.297	35.911	1.00	25.89
ATOM	736	NZ	LYS	94	32.998	1.075	35.012	1.00	28.49
ATOM	737	C	LYS	94	35.539	6.242	38.610	1.00	8.51
ATOM	738	O	LYS	94	36.749	6.036	38.748	1.00	6.81
ATOM	739	N	ILE	95	34.686	6.078	39.604	1.00	7.95
ATOM	740	CA	ILE	95	35.040	5.534	40.910	1.00	6.10
ATOM	741	CB	ILE	95	34.014	5.898	41.954	1.00	5.18
ATOM	742	CG1	ILE	95	34.046	7.444	42.211	1.00	6.06
ATOM	743	CD1	ILE	95	32.837	7.904	43.045	1.00	5.94
ATOM	744	CG2	ILE	95	34.329	5.157	43.281	1.00	5.58
ATOM	745	C	ILE	95	35.166	3.997	40.716	1.00	6.29
ATOM	746	O	ILE	95	34.198	3.309	40.347	1.00	5.34
ATOM	747	N	VAL	96	36.391	3.492	40.859	1.00	4.94
ATOM	748	CA	VAL	96	36.632	2.073	40.636	1.00	5.84
ATOM	749	CB	VAL	96	37.831	1.745	39.776	1.00	5.80
ATOM	750	CG1	VAL	96	37.679	2.310	38.351	1.00	6.24
ATOM	751	CG2	VAL	96	39.165	2.258	40.318	1.00	5.22
ATOM	752	C	VAL	96	36.608	1.295	41.950	1.00	5.83
ATOM	753	O	VAL	96	36.279	0.126	41.914	1.00	5.47
ATOM	754	N	SER	97	36.847	1.959	43.077	1.00	5.14
ATOM	755	CA	SER	97	36.830	1.376	44.383	1.00	5.56
ATOM	756	CB	SER	97	38.128	0.683	44.766	1.00	3.06

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	757	OG	SER	97	39.236	1.451	44.594	1.00	6.94
ATOM	758	C	SER	97	36.592	2.485	45.447	1.00	6.21
ATOM	759	O	SER	97	36.842	3.650	45.154	1.00	5.16
ATOM	760	N	HIS	98	36.080	2.045	46.577	1.00	5.51
ATOM	761	CA	HIS	98	35.807	2.912	47.695	1.00	6.19
ATOM	762	CB	HIS	98	34.521	3.705	47.410	1.00	5.68
ATOM	763	CG	HIS	98	33.314	2.839	47.189	1.00	3.10
ATOM	764	ND1	HIS	98	32.540	2.415	48.249	1.00	5.80
ATOM	765	CE1	HIS	98	31.533	1.690	47.820	1.00	3.91
ATOM	766	NE2	HIS	98	31.630	1.631	46.504	1.00	4.11
ATOM	767	CD2	HIS	98	32.731	2.333	46.100	1.00	2.55
ATOM	768	C	HIS	98	35.718	2.187	49.043	1.00	6.46
ATOM	769	O	HIS	98	35.484	0.998	49.174	1.00	5.57
ATOM	770	N	SER	99	35.882	2.968	50.123	1.00	6.76
ATOM	771	CA	SER	99	35.744	2.476	51.476	1.00	6.43
ATOM	772	CB	SER	99	36.188	3.588	52.459	1.00	7.38
ATOM	773	OG	SER	99	35.341	4.757	52.354	1.00	7.60
ATOM	774	C	SER	99	34.290	2.177	51.765	1.00	6.67
ATOM	775	O	SER	99	33.365	2.734	51.153	1.00	7.55
ATOM	776	N	VAL	100	34.005	1.310	52.714	1.00	6.58
ATOM	777	CA	VAL	100	32.615	1.043	53.160	1.00	6.28
ATOM	778	CB	VAL	100	32.598	-0.278	53.971	1.00	6.35
ATOM	779	CG1	VAL	100	31.215	-0.420	54.605	1.00	6.97
ATOM	780	CG2	VAL	100	32.745	-1.461	52.932	1.00	6.04
ATOM	781	C	VAL	100	32.175	2.219	54.062	1.00	6.51
ATOM	782	O	VAL	100	31.049	2.745	54.044	1.00	6.77
ATOM	783	N	GLN	101	33.124	2.741	54.816	1.00	7.40
ATOM	784	CA	GLN	101	32.865	3.871	55.734	1.00	9.68
ATOM	785	CB	GLN	101	34.012	4.032	56.704	1.00	9.29
ATOM	786	CG	GLN	101	33.909	5.192	57.649	1.00	9.97
ATOM	787	CD	GLN	101	35.017	5.329	58.642	1.00	10.63
ATOM	788	OE1	GLN	101	36.190	5.548	58.257	1.00	13.55
ATOM	789	NE2	GLN	101	34.656	5.267	59.887	1.00	11.28
ATOM	790	C	GLN	101	32.569	5.189	54.993	1.00	9.37
ATOM	791	O	GLN	101	33.236	5.551	54.068	1.00	7.54
ATOM	792	N	GLU	102	31.480	5.845	55.472	1.00	9.24
ATOM	793	CA	GLU	102	31.008	7.074	54.921	1.00	9.90
ATOM	794	CB	GLU	102	29.464	7.141	55.018	1.00	11.63
ATOM	795	CG	GLU	102	28.763	6.013	54.261	1.00	12.22
ATOM	796	CD	GLU	102	27.278	6.126	54.402	1.00	14.95

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	797	OE1	GLU	102	26.805	6.596	55.462	1.00	18.92
ATOM	798	OE2	GLU	102	26.511	5.770	53.500	1.00	16.02
ATOM	799	C	GLU	102	31.533	8.340	55.593	1.00	10.50
ATOM	800	O	GLU	102	32.169	8.275	56.630	1.00	11.22
ATOM	801	N	ALA	103	31.273	9.485	54.974	1.00	9.97
ATOM	802	CA	ALA	103	31.699	10.772	55.541	1.00	9.74
ATOM	803	CB	ALA	103	33.049	11.245	55.034	1.00	8.10
ATOM	804	C	ALA	103	30.644	11.816	55.123	1.00	9.71
ATOM	805	O	ALA	103	30.011	11.529	54.129	1.00	9.34
ATOM	806	N	TYR	104	30.556	12.936	55.808	1.00	9.87
ATOM	807	CA	TYR	104	29.585	13.984	55.438	1.00	11.04
ATOM	808	CB	TYR	104	28.192	13.707	56.083	1.00	11.01
ATOM	809	CG	TYR	104	28.273	13.737	57.596	1.00	12.87
ATOM	810	CD1	TYR	104	27.958	14.884	58.330	1.00	14.01
ATOM	811	CE1	TYR	104	28.088	14.909	59.727	1.00	13.96
ATOM	812	CZ	TYR	104	28.519	13.774	60.389	1.00	14.95
ATOM	813	OH	TYR	104	28.676	13.775	61.757	1.00	15.04
ATOM	814	CE2	TYR	104	28.796	12.619	59.685	1.00	13.61
ATOM	815	CD2	TYR	104	28.665	12.589	58.310	1.00	13.25
ATOM	816	C	TYR	104	30.135	15.342	55.885	1.00	10.66
ATOM	817	O	TYR	104	30.942	15.394	56.853	1.00	11.97
ATOM	818	N	LEU	105	29.819	16.416	55.227	1.00	10.31
ATOM	819	CA	LEU	105	30.271	17.775	55.675	1.00	10.31
ATOM	820	CB	LEU	105	30.363	18.745	54.499	1.00	8.28
ATOM	821	CG	LEU	105	31.202	18.355	53.295	1.00	7.12
ATOM	822	CD1	LEU	105	31.189	19.393	52.190	1.00	5.52
ATOM	823	CD2	LEU	105	32.669	18.076	53.663	1.00	5.12
ATOM	824	C	LEU	105	29.156	18.174	56.667	1.00	10.48
ATOM	825	O	LEU	105	27.977	17.998	56.358	1.00	10.24
ATOM	826	N	PRO	106	29.469	18.627	57.865	1.00	11.95
ATOM	827	CA	PRO	106	28.454	18.963	58.863	1.00	12.84
ATOM	828	CB	PRO	106	29.276	19.275	60.093	1.00	13.00
ATOM	829	CG	PRO	106	30.549	19.799	59.534	1.00	14.02
ATOM	830	CD	PRO	106	30.826	18.911	58.327	1.00	13.21
ATOM	831	C	PRO	106	27.479	20.038	58.465	1.00	13.69
ATOM	832	O	PRO	106	26.376	20.106	59.000	1.00	14.91
ATOM	833	N	THR	107	27.838	20.930	57.523	1.00	14.66
ATOM	834	CA	THR	107	26.983	21.976	57.008	1.00	16.19
ATOM	835	CB	THR	107	27.799	23.235	56.607	1.00	21.67
ATOM	836	OG1	THR	107	28.885	22.852	55.716	1.00	25.40

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	837	CG2	THR	107	28.349	23.915	57.844	1.00	24.07
ATOM	838	C	THR	107	26.199	21.591	55.752	1.00	13.84
ATOM	839	O	THR	107	25.549	22.430	55.155	1.00	14.95
ATOM	840	N	GLY	108	26.232	20.326	55.368	1.00	11.38
ATOM	841	CA	GLY	108	25.547	19.869	54.176	1.00	8.51
ATOM	842	C	GLY	108	26.402	20.337	53.000	1.00	7.43
ATOM	843	O	GLY	108	27.611	20.629	53.127	1.00	7.41
ATOM	844	N	GLU	109	25.808	20.388	51.837	1.00	6.61
ATOM	845	CA	GLU	109	26.466	20.806	50.634	1.00	7.52
ATOM	846	CB	GLU	109	26.686	19.615	49.685	1.00	7.66
ATOM	847	CG	GLU	109	27.582	18.521	50.288	1.00	5.52
ATOM	848	CD	GLU	109	27.731	17.381	49.320	1.00	7.26
ATOM	849	OE1	GLU	109	27.368	17.478	48.139	1.00	7.28
ATOM	850	OE2	GLU	109	28.195	16.298	49.739	1.00	8.58
ATOM	851	C	GLU	109	25.653	21.884	49.896	1.00	8.48
ATOM	852	O	GLU	109	24.554	22.191	50.241	1.00	10.22
ATOM	853	N	GLY	110	26.303	22.414	48.883	1.00	10.01
ATOM	854	CA	GLY	110	25.702	23.424	47.989	1.00	10.84
ATOM	855	C	GLY	110	26.178	23.098	46.548	1.00	11.21
ATOM	856	O	GLY	110	27.056	22.281	46.342	1.00	11.00
ATOM	857	N	CYS	111	25.608	23.776	45.582	1.00	11.21
ATOM	858	CA	CYS	111	25.870	23.582	44.163	1.00	10.09
ATOM	859	C	CYS	111	25.533	24.848	43.352	1.00	10.36
ATOM	860	O	CYS	111	24.562	25.536	43.627	1.00	10.29
ATOM	861	CB	CYS	111	24.923	22.434	43.721	1.00	9.84
ATOM	862	SG	CYS	111	25.048	21.924	42.045	1.00	8.95
ATOM	863	N	LEU	112	26.398	25.177	42.403	1.00	11.20
ATOM	864	CA	LEU	112	26.170	26.384	41.550	1.00	11.83
ATOM	865	CB	LEU	112	27.411	26.486	40.666	1.00	12.57
ATOM	866	CG	LEU	112	28.708	26.878	41.352	1.00	15.06
ATOM	867	CD1	LEU	112	29.871	26.352	40.469	1.00	15.77
ATOM	868	CD2	LEU	112	28.926	28.394	41.340	1.00	15.61
ATOM	869	C	LEU	112	24.851	26.350	40.836	1.00	11.60
ATOM	870	O	LEU	112	24.228	27.383	40.488	1.00	11.36
ATOM	871	N	SER	113	24.310	25.146	40.587	1.00	11.85
ATOM	872	CA	SER	113	23.048	24.950	39.917	1.00	11.15
ATOM	873	CB	SER	113	23.025	23.699	39.049	1.00	10.66
ATOM	874	OG	SER	113	23.968	23.793	37.992	1.00	7.38
ATOM	875	C	SER	113	21.886	24.945	40.885	1.00	12.54
ATOM	876	O	SER	113	20.731	24.917	40.427	1.00	14.05

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TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	877	N	VAL	114	22.143	24.975	42.198	1.00	11.90
ATOM	878	CA	VAL	114	21.022	25.016	43.143	1.00	11.54
ATOM	879	CB	VAL	114	21.067	23.872	44.160	1.00	9.05
ATOM	880	CG1	VAL	114	19.777	23.919	45.007	1.00	10.95
ATOM	881	CG2	VAL	114	21.080	22.538	43.409	1.00	9.28
ATOM	882	C	VAL	114	21.005	26.402	43.818	1.00	11.42
ATOM	883	O	VAL	114	21.854	26.663	44.630	1.00	11.25
ATOM	884	N	ASP	115	20.077	27.277	43.466	1.00	12.74
ATOM	885	CA	ASP	115	20.012	28.618	43.985	1.00	15.39
ATOM	886	CB	ASP	115	19.029	29.540	43.310	1.00	17.73
ATOM	887	CG	ASP	115	19.300	29.933	41.893	1.00	20.05
ATOM	888	OD1	ASP	115	20.331	29.598	41.312	1.00	18.80
ATOM	889	OD2	ASP	115	18.380	30.637	41.372	1.00	22.85
ATOM	890	C	ASP	115	19.789	28.760	45.492	1.00	16.27
ATOM	891	O	ASP	115	20.405	29.626	46.099	1.00	17.11
ATOM	892	N	ASP	116	18.857	28.001	46.028	1.00	17.25
ATOM	893	CA	ASP	116	18.590	28.081	47.461	1.00	18.90
ATOM	894	CB	ASP	116	17.117	27.717	47.739	1.00	21.30
ATOM	895	CG	ASP	116	16.153	28.650	47.041	1.00	24.14
ATOM	896	OD1	ASP	116	16.391	29.883	47.008	1.00	23.07
ATOM	897	OD2	ASP	116	15.132	28.134	46.495	1.00	26.77
ATOM	898	C	ASP	116	19.444	27.106	48.249	1.00	19.20
ATOM	899	O	ASP	116	19.738	26.025	47.744	1.00	19.78
ATOM	900	N	ASN	117	19.869	27.534	49.428	1.00	18.50
ATOM	901	CA	ASN	117	20.571	26.691	50.352	1.00	18.69
ATOM	902	CB	ASN	117	21.143	27.363	51.585	1.00	19.43
ATOM	903	CG	ASN	117	22.487	28.000	51.304	1.00	22.50
ATOM	904	OD1	ASN	117	23.330	27.263	50.736	1.00	23.16
ATOM	905	ND2	ASN	117	22.749	29.225	51.663	1.00	22.67
ATOM	906	C	ASN	117	19.655	25.543	50.781	1.00	19.22
ATOM	907	O	ASN	117	18.465	25.737	51.042	1.00	20.65
ATOM	908	N	VAL	118	20.216	24.324	50.775	1.00	18.92
ATOM	909	CA	VAL	118	19.445	23.151	51.178	1.00	18.04
ATOM	910	CB	VAL	118	19.364	22.090	50.077	1.00	18.23
ATOM	911	CG1	VAL	118	18.474	20.906	50.480	1.00	15.62
ATOM	912	CG2	VAL	118	18.797	22.712	48.813	1.00	18.51
ATOM	913	C	VAL	118	20.133	22.575	52.422	1.00	17.95
ATOM	914	O	VAL	118	21.338	22.351	52.430	1.00	17.23
ATOM	915	N	ALA	119	19.326	22.435	53.478	1.00	17.06
ATOM	916	CA	ALA	119	19.833	21.907	54.727	1.00	17.10

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	917	CB	ALA	119	18.932	22.450	55.851	1.00	17.38
ATOM	918	C	ALA	119	19.739	20.368	54.722	1.00	16.72
ATOM	919	O	ALA	119	18.760	19.858	54.161	1.00	16.13
ATOM	920	N	GLY	120	20.718	19.683	55.320	1.00	15.41
ATOM	921	CA	GLY	120	20.621	18.216	55.347	1.00	14.28
ATOM	922	C	GLY	120	21.960	17.576	55.058	1.00	13.76
ATOM	923	O	GLY	120	22.737	18.067	54.234	1.00	14.66
ATOM	924	N	LEU	121	22.244	16.452	55.717	1.00	12.70
ATOM	925	CA	LEU	121	23.529	15.767	55.522	1.00	11.00
ATOM	926	CB	LEU	121	23.882	15.004	56.781	1.00	10.76
ATOM	927	CG	LEU	121	23.943	15.759	58.103	1.00	9.49
ATOM	928	CD1	LEU	121	24.449	14.822	59.193	1.00	7.07
ATOM	929	CD2	LEU	121	24.866	16.971	57.969	1.00	8.49
ATOM	930	C	LEU	121	23.528	14.851	54.310	1.00	9.73
ATOM	931	O	LEU	121	22.575	14.134	53.975	1.00	10.55
ATOM	932	N	VAL	122	24.614	14.916	53.575	1.00	9.32
ATOM	933	CA	VAL	122	24.834	14.130	52.353	1.00	8.52
ATOM	934	CB	VAL	122	25.063	15.033	51.127	1.00	6.54
ATOM	935	CG1	VAL	122	25.255	14.183	49.858	1.00	6.34
ATOM	936	CG2	VAL	122	23.909	15.992	50.882	1.00	7.19
ATOM	937	C	VAL	122	26.025	13.196	52.613	1.00	8.38
ATOM	938	O	VAL	122	27.194	13.572	52.554	1.00	7.49
ATOM	939	N	HIS	123	25.693	11.961	52.933	1.00	8.70
ATOM	940	CA	HIS	123	26.619	10.910	53.254	1.00	9.15
ATOM	941	CB	HIS	123	25.995	9.863	54.141	1.00	8.55
ATOM	942	CG	HIS	123	25.490	10.280	55.476	1.00	8.68
ATOM	943	ND1	HIS	123	24.164	10.635	55.678	1.00	8.01
ATOM	944	CE1	HIS	123	23.986	10.913	56.974	1.00	7.33
ATOM	945	NE2	HIS	123	25.156	10.789	57.597	1.00	9.84
ATOM	946	CD2	HIS	123	26.079	10.374	56.687	1.00	8.51
ATOM	947	C	HIS	123	27.238	10.273	51.992	1.00	8.74
ATOM	948	O	HIS	123	26.548	9.818	51.133	1.00	9.79
ATOM	949	N	ARG	124	28.544	10.295	51.908	1.00	8.30
ATOM	950	CA	ARG	124	29.327	9.808	50.787	1.00	7.51
ATOM	951	CB	ARG	124	29.950	11.016	50.038	1.00	6.35
ATOM	952	CG	ARG	124	28.857	11.950	49.441	1.00	6.41
ATOM	953	CD	ARG	124	29.525	12.993	48.565	1.00	6.17
ATOM	954	NE	ARG	124	28.611	13.914	47.957	1.00	6.87
ATOM	955	CZ	ARG	124	27.747	13.824	46.996	1.00	8.12
ATOM	956	NH1	ARG	124	27.516	12.728	46.252	1.00	6.27

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	957	NH2	ARG	124	27.033	14.909	46.631	1.00	7.84
ATOM	958	C	ARG	124	30.408	8.871	51.264	1.00	7.13
ATOM	959	O	ARG	124	30.496	8.686	52.482	1.00	7.16
ATOM	960	N	HIS	125	31.238	8.287	50.388	1.00	8.38
ATOM	961	CA	HIS	125	32.302	7.401	50.830	1.00	9.33
ATOM	962	CB	HIS	125	32.816	6.389	49.794	1.00	9.69
ATOM	963	CG	HIS	125	31.660	5.665	49.141	1.00	7.74
ATOM	964	ND1	HIS	125	30.806	4.831	49.778	1.00	8.49
ATOM	965	CE1	HIS	125	29.907	4.383	48.933	1.00	7.96
ATOM	966	NE2	HIS	125	30.208	4.908	47.725	1.00	9.47
ATOM	967	CD2	HIS	125	31.289	5.714	47.836	1.00	8.48
ATOM	968	C	HIS	125	33.495	8.241	51.292	1.00	9.98
ATOM	969	O	HIS	125	33.868	9.228	50.668	1.00	11.12
ATOM	970	N	ASN	126	34.083	7.837	52.420	1.00	8.74
ATOM	971	CA	ASN	126	35.193	8.623	52.953	1.00	8.54
ATOM	972	CB	ASN	126	35.428	8.115	54.411	1.00	8.14
ATOM	973	CG	ASN	126	36.416	9.019	55.101	1.00	8.88
ATOM	974	OD1	ASN	126	36.270	10.238	54.953	1.00	10.54
ATOM	975	ND2	ASN	126	37.448	8.494	55.731	1.00	9.56
ATOM	976	C	ASN	126	36.402	8.566	52.090	1.00	8.32
ATOM	977	O	ASN	126	37.199	9.515	51.941	1.00	9.13
ATOM	978	N	LYS	127	36.595	7.416	51.408	1.00	8.46
ATOM	979	CA	LYS	127	37.733	7.182	50.536	1.00	6.93
ATOM	980	CB	LYS	127	38.785	6.232	51.138	1.00	8.23
ATOM	981	CG	LYS	127	39.335	6.671	52.443	1.00	13.12
ATOM	982	CD	LYS	127	40.489	5.811	52.965	1.00	16.68
ATOM	983	CE	LYS	127	40.871	6.388	54.335	1.00	21.82
ATOM	984	NZ	LYS	127	41.984	5.677	54.991	1.00	26.43
ATOM	985	C	LYS	127	37.279	6.566	49.206	1.00	5.67
ATOM	986	O	LYS	127	36.408	5.710	49.137	1.00	5.09
ATOM	987	N	ILE	128	37.890	7.084	48.137	1.00	6.06
ATOM	988	CA	ILE	128	37.584	6.599	46.802	1.00	5.35
ATOM	989	CB	ILE	128	36.554	7.482	46.060	1.00	3.79
ATOM	990	CG1	ILE	128	37.101	8.916	45.871	1.00	2.49
ATOM	991	CD1	ILE	128	36.165	9.779	45.033	1.00	4.28
ATOM	992	CG2	ILE	128	35.180	7.503	46.769	1.00	2.00
ATOM	993	C	ILE	128	38.855	6.553	45.951	1.00	4.84
ATOM	994	O	ILE	128	39.849	7.235	46.194	1.00	3.72
ATOM	995	N	THR	129	38.812	5.755	44.906	1.00	4.26
ATOM	996	CA	THR	129	39.886	5.639	43.932	1.00	5.44

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	997	CB	THR	129	40.600	4.262	43.874	1.00	5.74
ATOM	998	OG1	THR	129	41.384	4.124	45.083	1.00	6.67
ATOM	999	CG2	THR	129	41.546	4.171	42.697	1.00	3.87
ATOM	1000	C	THR	129	39.130	5.882	42.610	1.00	5.76
ATOM	1001	O	THR	129	38.104	5.237	42.387	1.00	4.96
ATOM	1002	N	ILE	130	39.584	6.856	41.882	1.00	6.40
ATOM	1003	CA	ILE	130	39.076	7.252	40.599	1.00	7.37
ATOM	1004	CB	ILE	130	38.692	8.769	40.544	1.00	7.11
ATOM	1005	CG1	ILE	130	37.391	8.969	41.370	1.00	7.19
ATOM	1006	CD1	ILE	130	36.998	10.444	41.506	1.00	10.30
ATOM	1007	CG2	ILE	130	38.474	9.320	39.150	1.00	7.49
ATOM	1008	C	ILE	130	40.132	7.022	39.492	1.00	7.21
ATOM	1009	O	ILE	130	41.291	7.322	39.617	1.00	6.63
ATOM	1010	N	LYS	131	39.603	6.521	38.372	1.00	7.02
ATOM	1011	CA	LYS	131	40.359	6.352	37.170	1.00	8.19
ATOM	1012	CB	LYS	131	40.513	4.982	36.602	1.00	11.33
ATOM	1013	CG	LYS	131	41.314	3.971	37.416	1.00	13.57
ATOM	1014	CD	LYS	131	41.458	2.749	36.505	1.00	17.15
ATOM	1015	CE	LYS	131	42.455	1.746	37.039	1.00	20.87
ATOM	1016	NZ	LYS	131	42.779	0.788	35.929	1.00	25.22
ATOM	1017	C	LYS	131	39.709	7.288	36.109	1.00	6.91
ATOM	1018	O	LYS	131	38.489	7.342	36.009	1.00	5.90
ATOM	1019	N	ALA	132	40.583	8.053	35.447	1.00	6.42
ATOM	1020	CA	ALA	132	40.013	8.945	34.400	1.00	5.33
ATOM	1021	CB	ALA	132	39.562	10.235	35.083	1.00	2.00
ATOM	1022	C	ALA	132	41.063	9.240	33.354	1.00	5.57
ATOM	1023	O	ALA	132	42.191	8.728	33.449	1.00	6.67
ATOM	1024	N	LYS	133	40.734	10.026	32.341	1.00	6.83
ATOM	1025	CA	LYS	133	41.758	10.489	31.375	1.00	7.84
ATOM	1026	CB	LYS	133	41.311	10.463	29.904	1.00	9.83
ATOM	1027	CG	LYS	133	40.878	9.164	29.336	1.00	11.29
ATOM	1028	CD	LYS	133	41.983	8.133	29.442	1.00	14.36
ATOM	1029	CE	LYS	133	41.577	6.842	28.727	1.00	16.88
ATOM	1030	NZ	LYS	133	42.601	5.811	29.133	1.00	17.94
ATOM	1031	C	LYS	133	41.887	12.006	31.643	1.00	6.97
ATOM	1032	O	LYS	133	40.940	12.600	32.143	1.00	7.81
ATOM	1033	N	ASP	134	42.949	12.623	31.268	1.00	8.29
ATOM	1034	CA	ASP	134	43.141	14.055	31.363	1.00	7.39
ATOM	1035	CB	ASP	134	44.519	14.454	31.823	1.00	8.51
ATOM	1036	CG	ASP	134	45.717	14.189	30.975	1.00	8.37

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	1037	OD1	ASP	134	46.894	14.220	31.413	1.00	8.77
ATOM	1038	OD2	ASP	134	45.585	13.946	29.746	1.00	9.62
ATOM	1039	C	ASP	134	42.752	14.675	30.015	1.00	9.13
ATOM	1040	O	ASP	134	42.283	13.980	29.053	1.00	10.00
ATOM	1041	N	ILE	135	42.905	15.962	29.856	1.00	8.82
ATOM	1042	CA	ILE	135	42.538	16.710	28.635	1.00	9.79
ATOM	1043	CB	ILE	135	42.652	18.224	28.949	1.00	10.08
ATOM	1044	CG1	ILE	135	41.900	19.058	27.938	1.00	9.25
ATOM	1045	CD1	ILE	135	41.972	20.551	28.227	1.00	9.86
ATOM	1046	CG2	ILE	135	44.134	18.642	28.921	1.00	10.69
ATOM	1047	C	ILE	135	43.229	16.263	27.395	1.00	9.88
ATOM	1048	O	ILE	135	42.729	16.310	26.254	1.00	10.08
ATOM	1049	N	GLU	136	44.447	15.717	27.490	1.00	9.82
ATOM	1050	CA	GLU	136	45.211	15.168	26.423	1.00	9.97
ATOM	1051	CB	GLU	136	46.721	15.501	26.503	1.00	9.18
ATOM	1052	CG	GLU	136	47.025	16.963	26.269	1.00	11.11
ATOM	1053	CD	GLU	136	46.573	17.426	24.871	1.00	11.43
ATOM	1054	OE1	GLU	136	46.759	16.636	23.938	1.00	12.83
ATOM	1055	OE2	GLU	136	46.039	18.527	24.823	1.00	12.16
ATOM	1056	C	GLU	136	45.033	13.647	26.240	1.00	9.67
ATOM	1057	O	GLU	136	45.793	13.083	25.431	1.00	10.16
ATOM	1058	N	GLY	137	44.149	12.996	26.990	1.00	8.60
ATOM	1059	CA	GLY	137	43.916	11.554	26.862	1.00	7.80
ATOM	1060	C	GLY	137	44.812	10.661	27.640	1.00	6.10
ATOM	1061	O	GLY	137	44.951	9.443	27.445	1.00	6.27
ATOM	1062	N	ASN	138	45.611	11.224	28.533	1.00	6.53
ATOM	1063	CA	ASN	138	46.540	10.485	29.348	1.00	7.17
ATOM	1064	CB	ASN	138	47.859	11.112	29.564	1.00	6.62
ATOM	1065	CG	ASN	138	48.666	11.343	28.324	1.00	6.41
ATOM	1066	OD1	ASN	138	48.891	10.474	27.473	1.00	7.83
ATOM	1067	ND2	ASN	138	49.080	12.589	28.118	1.00	5.84
ATOM	1068	C	ASN	138	45.782	9.938	30.557	1.00	8.75
ATOM	1069	O	ASN	138	44.731	10.431	30.900	1.00	9.34
ATOM	1070	N	ASP	139	46.289	8.893	31.200	1.00	9.51
ATOM	1071	CA	ASP	139	45.642	8.232	32.304	1.00	9.46
ATOM	1072	CB	ASP	139	46.137	6.738	32.368	1.00	9.74
ATOM	1073	CG	ASP	139	45.953	6.042	31.034	1.00	10.25
ATOM	1074	OD1	ASP	139	45.029	6.416	30.295	1.00	10.01
ATOM	1075	OD2	ASP	139	46.802	5.192	30.714	1.00	10.42
ATOM	1076	C	ASP	139	45.931	8.866	33.648	1.00	8.48

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TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	1077	O	ASP	139	47.094	9.212	33.934	1.00	8.89
ATOM	1078	N	ILE	140	44.896	9.015	34.458	1.00	8.07
ATOM	1079	CA	ILE	140	45.072	9.590	35.799	1.00	9.43
ATOM	1080	CB	ILE	140	44.435	10.979	35.964	1.00	12.18
ATOM	1081	CG1	ILE	140	44.723	11.979	34.883	1.00	15.73
ATOM	1082	CD1	ILE	140	46.188	12.373	34.669	1.00	17.79
ATOM	1083	CG2	ILE	140	44.881	11.612	37.311	1.00	13.76
ATOM	1084	C	ILE	140	44.358	8.632	36.775	1.00	8.12
ATOM	1085	O	ILE	140	43.265	8.238	36.565	1.00	7.55
ATOM	1086	N	GLN	141	44.992	8.330	37.908	1.00	8.68
ATOM	1087	CA	GLN	141	44.370	7.492	38.929	1.00	8.09
ATOM	1088	CB	GLN	141	44.930	6.081	39.016	1.00	10.14
ATOM	1089	CG	GLN	141	44.139	5.210	39.984	1.00	13.25
ATOM	1090	CD	GLN	141	44.556	3.767	40.096	1.00	14.70
ATOM	1091	OE1	GLN	141	45.723	3.425	40.103	1.00	16.12
ATOM	1092	NE2	GLN	141	43.607	2.851	40.176	1.00	14.82
ATOM	1093	C	GLN	141	44.575	8.281	40.247	1.00	6.14
ATOM	1094	O	GLN	141	45.713	8.595	40.573	1.00	7.17
ATOM	1095	N	LEU	142	43.498	8.589	40.928	1.00	4.24
ATOM	1096	CA	LEU	142	43.540	9.376	42.127	1.00	4.16
ATOM	1097	CB	LEU	142	42.641	10.638	42.092	1.00	3.14
ATOM	1098	CG	LEU	142	42.865	11.671	40.964	1.00	4.72
ATOM	1099	CD1	LEU	142	42.418	11.139	39.628	1.00	7.12
ATOM	1100	CD2	LEU	142	42.191	12.984	41.303	1.00	5.38
ATOM	1101	C	LEU	142	43.024	8.590	43.362	1.00	4.55
ATOM	1102	O	LEU	142	42.026	7.918	43.302	1.00	3.43
ATOM	1103	N	ARG	143	43.706	8.838	44.442	1.00	5.60
ATOM	1104	CA	ARG	143	43.254	8.230	45.735	1.00	6.45
ATOM	1105	CB	ARG	143	44.406	7.410	46.295	1.00	6.30
ATOM	1106	CG	ARG	143	44.572	6.089	45.510	1.00	6.38
ATOM	1107	CD	ARG	143	45.870	5.421	45.955	1.00	7.24
ATOM	1108	NE	ARG	143	46.994	6.164	45.399	1.00	8.41
ATOM	1109	CZ	ARG	143	47.487	6.175	44.186	1.00	7.10
ATOM	1110	NH1	ARG	143	47.010	5.371	43.229	1.00	10.56
ATOM	1111	NH2	ARG	143	48.441	6.994	43.872	1.00	6.66
ATOM	1112	C	ARG	143	42.862	9.416	46.587	1.00	6.59
ATOM	1113	O	ARG	143	43.759	10.213	46.872	1.00	8.32
ATOM	1114	N	LEU	144	41.608	9.616	46.887	1.00	6.29
ATOM	1115	CA	LEU	144	41.146	10.800	47.621	1.00	7.40
ATOM	1116	CB	LEU	144	40.077	11.501	46.737	1.00	8.55

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TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	1117	CG	LEU	144	40.603	12.027	45.375	1.00	8.47
ATOM	1118	CD1	LEU	144	39.402	12.282	44.481	1.00	6.95
ATOM	1119	CD2	LEU	144	41.379	13.312	45.591	1.00	5.70
ATOM	1120	C	LEU	144	40.470	10.405	48.909	1.00	9.13
ATOM	1121	O	LEU	144	39.953	9.293	49.040	1.00	8.94
ATOM	1122	N	LYS	145	40.423	11.365	49.832	1.00	10.82
ATOM	1123	CA	LYS	145	39.801	11.116	51.142	1.00	11.39
ATOM	1124	CB	LYS	145	40.924	10.619	52.041	1.00	13.95
ATOM	1125	CG	LYS	145	40.646	10.374	53.458	1.00	18.80
ATOM	1126	CD	LYS	145	41.861	9.909	54.232	1.00	25.06
ATOM	1127	CE	LYS	145	42.963	10.908	54.354	1.00	31.66
ATOM	1128	NZ	LYS	145	43.539	11.396	53.059	1.00	37.64
ATOM	1129	C	LYS	145	39.188	12.388	51.720	1.00	9.96
ATOM	1130	O	LYS	145	39.596	13.478	51.389	1.00	9.17
ATOM	1131	N	GLY	146	38.108	12.225	52.519	1.00	8.79
ATOM	1132	CA	GLY	146	37.456	13.328	53.137	1.00	8.43
ATOM	1133	C	GLY	146	36.897	14.360	52.201	1.00	8.40
ATOM	1134	O	GLY	146	36.151	14.060	51.254	1.00	8.45
ATOM	1135	N	TYR	147	37.263	15.616	52.405	1.00	8.09
ATOM	1136	CA	TYR	147	36.779	16.715	51.642	1.00	7.87
ATOM	1137	CB	TYR	147	37.196	18.074	52.234	1.00	9.36
ATOM	1138	CG	TYR	147	36.595	19.261	51.474	1.00	11.07
ATOM	1139	CD1	TYR	147	35.277	19.634	51.672	1.00	11.07
ATOM	1140	CE1	TYR	147	34.748	20.679	50.935	1.00	13.45
ATOM	1141	CZ	TYR	147	35.529	21.400	50.057	1.00	13.62
ATOM	1142	OH	TYR	147	35.036	22.483	49.389	1.00	13.97
ATOM	1143	CE2	TYR	147	36.866	21.045	49.873	1.00	13.40
ATOM	1144	CD2	TYR	147	37.362	19.974	50.592	1.00	12.10
ATOM	1145	C	TYR	147	36.885	16.626	50.152	1.00	5.90
ATOM	1146	O	TYR	147	35.845	16.786	49.504	1.00	4.84
ATOM	1147	N	PRO	148	38.043	16.403	49.590	1.00	7.00
ATOM	1148	CA	PRO	148	38.156	16.303	48.132	1.00	7.78
ATOM	1149	CB	PRO	148	39.605	16.180	47.837	1.00	7.31
ATOM	1150	CG	PRO	148	40.271	15.930	49.125	1.00	8.35
ATOM	1151	CD	PRO	148	39.340	16.286	50.255	1.00	7.21
ATOM	1152	C	PRO	148	37.394	15.074	47.639	1.00	7.01
ATOM	1153	O	PRO	148	36.995	15.119	46.479	1.00	8.08
ATOM	1154	N	ALA	149	37.271	14.025	48.435	1.00	5.19
ATOM	1155	CA	ALA	149	36.571	12.828	48.000	1.00	4.31
ATOM	1156	CB	ALA	149	36.715	11.666	48.983	1.00	2.00

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	1157	C	ALA	149	35.079	13.175	47.824	1.00	3.82
ATOM	1158	O	ALA	149	34.463	12.772	46.850	1.00	3.79
ATOM	1159	N	ILE	150	34.535	13.957	48.742	1.00	4.49
ATOM	1160	CA	ILE	150	33.146	14.400	48.705	1.00	5.37
ATOM	1161	CB	ILE	150	32.790	15.107	50.026	1.00	7.40
ATOM	1162	CG2	ILE	150	31.624	16.049	49.837	1.00	7.23
ATOM	1163	CG1	ILE	150	32.660	14.085	51.137	1.00	8.06
ATOM	1164	CD1	ILE	150	32.623	14.512	52.578	1.00	7.31
ATOM	1165	C	ILE	150	32.925	15.337	47.504	1.00	4.53
ATOM	1166	O	ILE	150	31.943	15.147	46.813	1.00	3.53
ATOM	1167	N	VAL	151	33.896	16.213	47.249	1.00	4.55
ATOM	1168	CA	VAL	151	33.781	17.130	46.083	1.00	4.71
ATOM	1169	CB	VAL	151	34.800	18.238	46.088	1.00	4.83
ATOM	1170	CG1	VAL	151	34.777	19.142	44.820	1.00	4.32
ATOM	1171	CG2	VAL	151	34.475	19.164	47.311	1.00	5.52
ATOM	1172	C	VAL	151	33.820	16.304	44.795	1.00	5.66
ATOM	1173	O	VAL	151	32.961	16.581	43.957	1.00	6.35
ATOM	1174	N	PHE	152	34.749	15.379	44.629	1.00	4.24
ATOM	1175	CA	PHE	152	34.658	14.562	43.361	1.00	4.96
ATOM	1176	CB	PHE	152	35.902	13.806	43.085	1.00	4.05
ATOM	1177	CG	PHE	152	37.140	14.561	42.669	1.00	6.55
ATOM	1178	CD1	PHE	152	37.911	15.246	43.583	1.00	7.52
ATOM	1179	CE1	PHE	152	39.104	15.892	43.234	1.00	6.30
ATOM	1180	CZ	PHE	152	39.474	15.858	41.904	1.00	4.29
ATOM	1181	CE2	PHE	152	38.732	15.203	40.973	1.00	3.38
ATOM	1182	CD2	PHE	152	37.586	14.528	41.355	1.00	4.89
ATOM	1183	C	PHE	152	33.386	13.735	43.308	1.00	4.69
ATOM	1184	O	PHE	152	32.812	13.579	42.203	1.00	5.23
ATOM	1185	N	GLN	153	32.847	13.159	44.374	1.00	4.19
ATOM	1186	CA	GLN	153	31.588	12.395	44.269	1.00	5.10
ATOM	1187	CB	GLN	153	31.284	11.638	45.555	1.00	4.46
ATOM	1188	CG	GLN	153	32.324	10.564	45.854	1.00	5.68
ATOM	1189	CD	GLN	153	32.214	9.837	47.177	1.00	7.54
ATOM	1190	OE1	GLN	153	31.475	8.874	47.401	1.00	9.94
ATOM	1191	NE2	GLN	153	33.031	10.289	48.117	1.00	5.48
ATOM	1192	C	GLN	153	30.446	13.259	43.812	1.00	5.17
ATOM	1193	O	GLN	153	29.581	12.883	42.981	1.00	6.71
ATOM	1194	N	HIS	154	30.385	14.471	44.338	1.00	4.09
ATOM	1195	CA	HIS	154	29.340	15.431	43.990	1.00	4.25
ATOM	1196	CB	HIS	154	29.636	16.731	44.863	1.00	3.87

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	1197	CG	HIS	154	28.693	17.851	44.588	1.00	3.28
ATOM	1198	ND1	HIS	154	27.711	18.274	45.436	1.00	5.34
ATOM	1199	CE1	HIS	154	27.004	19.245	44.925	1.00	4.80
ATOM	1200	NE2	HIS	154	27.491	19.463	43.683	1.00	6.11
ATOM	1201	CD2	HIS	154	28.529	18.603	43.465	1.00	5.20
ATOM	1202	C	HIS	154	29.391	15.728	42.477	1.00	3.83
ATOM	1203	O	HIS	154	28.401	15.710	41.793	1.00	3.56
ATOM	1204	N	GLU	155	30.571	16.019	41.951	1.00	4.91
ATOM	1205	CA	GLU	155	30.779	16.302	40.553	1.00	7.09
ATOM	1206	CB	GLU	155	32.150	16.925	40.264	1.00	7.65
ATOM	1207	CG	GLU	155	32.331	18.281	41.029	1.00	6.88
ATOM	1208	CD	GLU	155	31.161	19.223	40.725	1.00	8.48
ATOM	1209	OE1	GLU	155	30.644	19.235	39.570	1.00	6.97
ATOM	1210	OE2	GLU	155	30.704	19.907	41.673	1.00	9.81
ATOM	1211	C	GLU	155	30.481	15.079	39.675	1.00	6.80
ATOM	1212	O	GLU	155	29.815	15.254	38.625	1.00	7.83
ATOM	1213	N	ILE	156	30.914	13.904	40.026	1.00	6.49
ATOM	1214	CA	ILE	156	30.573	12.698	39.226	1.00	6.27
ATOM	1215	CB	ILE	156	31.359	11.470	39.668	1.00	5.97
ATOM	1216	CG1	ILE	156	32.848	11.653	39.436	1.00	4.24
ATOM	1217	CD1	ILE	156	33.760	10.571	39.861	1.00	3.82
ATOM	1218	CG2	ILE	156	30.804	10.186	39.036	1.00	7.37
ATOM	1219	C	ILE	156	29.066	12.513	39.298	1.00	5.98
ATOM	1220	O	ILE	156	28.467	12.196	38.252	1.00	5.77
ATOM	1221	N	ASP	157	28.408	12.644	40.429	1.00	5.23
ATOM	1222	CA	ASP	157	26.978	12.553	40.507	1.00	5.85
ATOM	1223	CB	ASP	157	26.371	12.978	41.821	1.00	7.42
ATOM	1224	CG	ASP	157	26.314	11.911	42.878	1.00	10.11
ATOM	1225	OD1	ASP	157	26.594	10.731	42.577	1.00	9.03
ATOM	1226	OD2	ASP	157	25.822	12.253	43.982	1.00	10.69
ATOM	1227	C	ASP	157	26.248	13.307	39.386	1.00	7.07
ATOM	1228	O	ASP	157	25.287	12.755	38.834	1.00	8.10
ATOM	1229	N	HIS	158	26.661	14.502	39.062	1.00	6.19
ATOM	1230	CA	HIS	158	26.112	15.287	38.029	1.00	7.49
ATOM	1231	CB	HIS	158	26.810	16.641	37.753	1.00	5.85
ATOM	1232	CG	HIS	158	26.559	17.707	38.769	1.00	5.01
ATOM	1233	ND1	HIS	158	25.266	18.168	38.959	1.00	5.03
ATOM	1234	CE1	HIS	158	25.282	19.121	39.895	1.00	4.19
ATOM	1235	NE2	HIS	158	26.557	19.288	40.292	1.00	4.26
ATOM	1236	CD2	HIS	158	27.363	18.439	39.584	1.00	2.60

ATOM	1237	C	HIS	158	26.090	14.599	36.656	1.00	8.47
ATOM	1238	O	HIS	158	25.171	14.898	35.913	1.00	9.43
ATOM	1239	N	LEU	159	27.078	13.780	36.392	1.00	8.63
ATOM	1240	CA	LEU	159	27.220	13.074	35.122	1.00	9.33
ATOM	1241	CB	LEU	159	28.636	12.532	34.967	1.00	7.47
ATOM	1242	CG	LEU	159	29.853	13.426	35.128	1.00	7.64
ATOM	1243	CD1	LEU	159	31.101	12.606	34.923	1.00	6.21
ATOM	1244	CD2	LEU	159	29.832	14.677	34.295	1.00	6.97
ATOM	1245	C	LEU	159	26.192	11.937	35.024	1.00	8.64
ATOM	1246	O	LEU	159	25.885	11.426	33.947	1.00	7.94
ATOM	1247	N	ASN	160	25.605	11.583	36.164	1.00	9.77
ATOM	1248	CA	ASN	160	24.580	10.573	36.277	1.00	9.90
ATOM	1249	CB	ASN	160	24.944	9.490	37.318	1.00	10.05
ATOM	1250	CG	ASN	160	26.211	8.761	36.969	1.00	8.81
ATOM	1251	OD1	ASN	160	26.495	8.464	35.805	1.00	8.76
ATOM	1252	ND2	ASN	160	27.049	8.507	37.960	1.00	11.57
ATOM	1253	C	ASN	160	23.207	11.100	36.542	1.00	10.13
ATOM	1254	O	ASN	160	22.238	10.334	36.824	1.00	9.97
ATOM	1255	N	GLY	161	22.996	12.404	36.413	1.00	10.67
ATOM	1256	CA	GLY	161	21.695	13.015	36.647	1.00	9.90
ATOM	1257	C	GLY	161	21.275	13.057	38.096	1.00	10.81
ATOM	1258	O	GLY	161	20.049	13.064	38.394	1.00	11.80
ATOM	1259	N	VAL	162	22.196	13.066	39.037	1.00	10.62
ATOM	1260	CA	VAL	162	21.975	13.082	40.469	1.00	10.24
ATOM	1261	CB	VAL	162	22.883	11.980	41.119	1.00	12.28
ATOM	1262	CG1	VAL	162	22.819	12.009	42.654	1.00	11.36
ATOM	1263	CG2	VAL	162	22.436	10.623	40.619	1.00	10.82
ATOM	1264	C	VAL	162	22.378	14.419	41.070	1.00	9.72
ATOM	1265	O	VAL	162	23.480	14.919	40.817	1.00	9.92
ATOM	1266	N	MET	163	21.507	14.997	41.900	1.00	8.97
ATOM	1267	CA	MET	163	21.754	16.260	42.575	1.00	9.40
ATOM	1268	CB	MET	163	20.557	17.207	42.379	1.00	9.97
ATOM	1269	CG	MET	163	20.282	17.521	40.923	1.00	11.50
ATOM	1270	SD	MET	163	21.495	18.562	40.125	1.00	12.73
ATOM	1271	CE	MET	163	21.165	20.109	40.910	1.00	11.88
ATOM	1272	C	MET	163	22.009	15.970	44.058	1.00	10.17
ATOM	1273	O	MET	163	21.477	14.989	44.595	1.00	10.49
ATOM	1274	N	PHE	164	22.853	16.760	44.715	1.00	9.65
ATOM	1275	CA	PHE	164	23.213	16.489	46.086	1.00	8.95
ATOM	1276	CB	PHE	164	24.153	17.529	46.683	1.00	8.12

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	1277	CG	PHE	164	23.519	18.850	47.009	1.00	7.63
ATOM	1278	CD1	PHE	164	22.981	19.041	48.271	1.00	7.03
ATOM	1279	CD2	PHE	164	23.442	19.870	46.055	1.00	6.36
ATOM	1280	CE1	PHE	164	22.357	20.248	48.597	1.00	9.27
ATOM	1281	CE2	PHE	164	22.792	21.030	46.358	1.00	7.45
ATOM	1282	CZ	PHE	164	22.288	21.248	47.613	1.00	7.70
ATOM	1283	C	PHE	164	22.073	16.212	47.048	1.00	8.66
ATOM	1284	O	PHE	164	22.221	15.427	47.999	1.00	8.17
ATOM	1285	N	TYR	165	20.984	16.929	46.869	1.00	9.74
ATOM	1286	CA	TYR	165	19.833	16.874	47.754	1.00	9.53
ATOM	1287	CB	TYR	165	18.975	18.140	47.553	1.00	10.74
ATOM	1288	CG	TYR	165	18.393	18.301	46.175	1.00	9.43
ATOM	1289	CD1	TYR	165	17.319	17.501	45.785	1.00	9.93
ATOM	1290	CE1	TYR	165	16.744	17.616	44.529	1.00	9.33
ATOM	1291	CZ	TYR	165	17.210	18.604	43.679	1.00	8.93
ATOM	1292	OH	TYR	165	16.640	18.714	42.431	1.00	11.39
ATOM	1293	CE2	TYR	165	18.278	19.393	44.033	1.00	7.81
ATOM	1294	CD2	TYR	165	18.833	19.277	45.291	1.00	8.68
ATOM	1295	C	TYR	165	19.036	15.621	47.637	1.00	11.52
ATOM	1296	O	TYR	165	18.088	15.381	48.431	1.00	12.08
ATOM	1297	N	ASP	166	19.358	14.814	46.616	1.00	10.44
ATOM	1298	CA	ASP	166	18.686	13.533	46.441	1.00	10.72
ATOM	1299	CB	ASP	166	19.095	12.916	45.117	1.00	11.36
ATOM	1300	CG	ASP	166	18.738	13.691	43.871	1.00	12.08
ATOM	1301	OD1	ASP	166	17.862	14.574	43.837	1.00	13.05
ATOM	1302	OD2	ASP	166	19.284	13.344	42.800	1.00	12.90
ATOM	1303	C	ASP	166	19.152	12.599	47.567	1.00	10.61
ATOM	1304	O	ASP	166	18.499	11.577	47.834	1.00	9.33
ATOM	1305	N	HIS	167	20.291	12.921	48.205	1.00	10.36
ATOM	1306	CA	HIS	167	20.793	12.039	49.255	1.00	11.38
ATOM	1307	CB	HIS	167	22.358	12.033	49.264	1.00	10.95
ATOM	1308	CG	HIS	167	22.964	11.631	47.957	1.00	13.93
ATOM	1309	ND1	HIS	167	22.923	10.334	47.453	1.00	13.92
ATOM	1310	CE1	HIS	167	23.546	10.300	46.291	1.00	13.33
ATOM	1311	NE2	HIS	167	24.004	11.501	46.018	1.00	12.92
ATOM	1312	CD2	HIS	167	23.645	12.366	47.027	1.00	13.06
ATOM	1313	C	HIS	167	20.362	12.372	50.662	1.00	12.37
ATOM	1314	O	HIS	167	20.858	11.734	51.630	1.00	13.63
ATOM	1315	N	ILE	168	19.525	13.362	50.860	1.00	12.97
ATOM	1316	CA	ILE	168	19.109	13.854	52.159	1.00	12.73

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	1317	CB	ILE	168	18.951	15.425	52.054	1.00	13.57
ATOM	1318	CG1	ILE	168	20.228	16.110	51.593	1.00	11.58
ATOM	1319	CD1	ILE	168	20.226	17.595	51.292	1.00	10.84
ATOM	1320	CG2	ILE	168	18.502	15.964	53.420	1.00	12.92
ATOM	1321	C	ILE	168	17.838	13.216	52.672	1.00	14.26
ATOM	1322	O	ILE	168	16.805	13.155	52.017	1.00	15.10
ATOM	1323	N	ASP	169	17.823	12.772	53.913	1.00	15.41
ATOM	1324	CA	ASP	169	16.631	12.138	54.507	1.00	16.46
ATOM	1325	CB	ASP	169	17.078	11.500	55.840	1.00	16.03
ATOM	1326	CG	ASP	169	15.931	10.619	56.316	1.00	17.04
ATOM	1327	OD1	ASP	169	14.943	11.119	56.861	1.00	18.29
ATOM	1328	OD2	ASP	169	16.030	9.434	55.962	1.00	17.14
ATOM	1329	C	ASP	169	15.552	13.189	54.714	1.00	17.91
ATOM	1330	O	ASP	169	15.803	14.268	55.270	1.00	16.68
ATOM	1331	N	LYS	170	14.353	12.945	54.189	1.00	20.44
ATOM	1332	CA	LYS	170	13.289	13.920	54.322	1.00	24.90
ATOM	1333	CB	LYS	170	11.953	13.478	53.630	1.00	28.24
ATOM	1334	CG	LYS	170	10.958	14.663	53.604	1.00	31.46
ATOM	1335	CD	LYS	170	9.539	14.285	53.173	1.00	32.94
ATOM	1336	CE	LYS	170	8.812	13.500	54.256	1.00	33.30
ATOM	1337	NZ	LYS	170	7.402	13.165	53.899	1.00	34.02
ATOM	1338	C	LYS	170	12.943	14.155	55.804	1.00	25.11
ATOM	1339	O	LYS	170	12.858	15.277	56.264	1.00	26.53
ATOM	1340	N	ASP	171	12.768	13.048	56.520	1.00	24.81
ATOM	1341	CA	ASP	171	12.371	13.086	57.912	1.00	25.10
ATOM	1342	CB	ASP	171	11.725	11.776	58.342	1.00	29.27
ATOM	1343	CG	ASP	171	10.592	11.235	57.534	1.00	31.17
ATOM	1344	OD1	ASP	171	9.713	11.934	57.004	1.00	31.40
ATOM	1345	OD2	ASP	171	10.606	9.961	57.381	1.00	34.11
ATOM	1346	C	ASP	171	13.414	13.491	58.919	1.00	23.57
ATOM	1347	O	ASP	171	13.096	14.249	59.861	1.00	23.55
ATOM	1348	N	HIS	172	14.650	13.038	58.756	1.00	21.67
ATOM	1349	CA	HIS	172	15.718	13.379	59.697	1.00	19.37
ATOM	1350	CB	HIS	172	16.113	12.098	60.464	1.00	21.26
ATOM	1351	CG	HIS	172	14.941	11.559	61.215	1.00	23.69
ATOM	1352	ND1	HIS	172	14.618	12.008	62.472	1.00	24.87
ATOM	1353	CE1	HIS	172	13.515	11.392	62.882	1.00	26.42
ATOM	1354	NE2	HIS	172	13.139	10.532	61.925	1.00	26.64
ATOM	1355	CD2	HIS	172	14.026	10.625	60.873	1.00	25.35
ATOM	1356	C	HIS	172	16.950	13.850	58.932	1.00	16.97

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	1357	O	HIS	172	17.981	13.177	58.955	1.00	16.83
ATOM	1358	N	PRO	173	16.836	14.984	58.274	1.00	14.57
ATOM	1359	CA	PRO	173	17.899	15.518	57.452	1.00	13.11
ATOM	1360	CB	PRO	173	17.279	16.758	56.843	1.00	12.46
ATOM	1361	CG	PRO	173	16.198	17.136	57.826	1.00	12.80
ATOM	1362	CD	PRO	173	15.585	15.805	58.221	1.00	13.20
ATOM	1363	C	PRO	173	19.199	15.766	58.159	1.00	13.01
ATOM	1364	O	PRO	173	20.244	15.711	57.538	1.00	12.71
ATOM	1365	N	LEU	174	19.213	16.071	59.457	1.00	13.35
ATOM	1366	CA	LEU	174	20.415	16.341	60.183	1.00	13.25
ATOM	1367	CB	LEU	174	20.352	17.642	60.973	1.00	14.23
ATOM	1368	CG	LEU	174	20.025	18.898	60.156	1.00	13.91
ATOM	1369	CD1	LEU	174	20.038	20.108	61.077	1.00	16.72
ATOM	1370	CD2	LEU	174	20.967	19.113	58.996	1.00	15.55
ATOM	1371	C	LEU	174	20.917	15.204	61.019	1.00	14.24
ATOM	1372	O	LEU	174	21.890	15.390	61.748	1.00	14.10
ATOM	1373	N	GLN	175	20.363	14.016	60.855	1.00	15.52
ATOM	1374	CA	GLN	175	20.798	12.832	61.630	1.00	17.11
ATOM	1375	CB	GLN	175	19.623	11.857	61.795	1.00	20.95
ATOM	1376	CG	GLN	175	19.941	10.655	62.677	1.00	27.18
ATOM	1377	CD	GLN	175	18.877	9.585	62.700	1.00	31.22
ATOM	1378	OE1	GLN	175	18.540	8.994	63.751	1.00	33.20
ATOM	1379	NE2	GLN	175	18.330	9.235	61.533	1.00	33.65
ATOM	1380	C	GLN	175	21.922	12.122	60.898	1.00	16.99
ATOM	1381	O	GLN	175	21.713	11.588	59.798	1.00	16.15
ATOM	1382	N	PRO	176	23.104	12.137	61.448	1.00	17.92
ATOM	1383	CA	PRO	176	24.264	11.514	60.860	1.00	19.07
ATOM	1384	CB	PRO	176	25.425	11.958	61.729	1.00	18.77
ATOM	1385	CG	PRO	176	24.866	13.138	62.518	1.00	18.47
ATOM	1386	CD	PRO	176	23.452	12.771	62.748	1.00	17.86
ATOM	1387	C	PRO	176	24.188	9.990	60.900	1.00	20.17
ATOM	1388	O	PRO	176	23.732	9.400	61.895	1.00	20.92
ATOM	1389	N	HIS	177	24.619	9.352	59.807	1.00	19.53
ATOM	1390	CA	HIS	177	24.656	7.914	59.784	1.00	20.36
ATOM	1391	CB	HIS	177	24.919	7.206	58.469	1.00	18.20
ATOM	1392	CG	HIS	177	23.802	7.337	57.474	1.00	14.95
ATOM	1393	ND1	HIS	177	24.005	7.159	56.138	1.00	16.40
ATOM	1394	CE1	HIS	177	22.864	7.356	55.480	1.00	16.26
ATOM	1395	NE2	HIS	177	21.958	7.707	56.368	1.00	16.00
ATOM	1396	CD2	HIS	177	22.523	7.700	57.617	1.00	14.21

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	1397	C	HIS	177	25.658	7.423	60.841	1.00	21.02
ATOM	1398	O	HIS	177	26.693	8.019	61.082	1.00	22.02
ATOM	1399	N	THR	178	25.255	6.325	61.480	1.00	22.22
ATOM	1400	CA	THR	178	26.106	5.744	62.510	1.00	23.81
ATOM	1401	CB	THR	178	25.412	4.447	63.017	1.00	26.92
ATOM	1402	OG1	THR	178	24.070	4.779	63.455	1.00	28.11
ATOM	1403	CG2	THR	178	26.218	3.926	64.192	1.00	27.70
ATOM	1404	C	THR	178	27.479	5.379	61.959	1.00	23.54
ATOM	1405	O	THR	178	27.595	4.594	61.005	1.00	25.27
ATOM	1406	N	ASP	179	28.540	5.880	62.536	1.00	22.85
ATOM	1407	CA	ASP	179	29.901	5.593	62.172	1.00	22.95
ATOM	1408	CB	ASP	179	30.170	4.097	62.080	1.00	28.84
ATOM	1409	CG	ASP	179	29.950	3.241	63.312	1.00	33.14
ATOM	1410	OD1	ASP	179	29.420	2.094	63.173	1.00	34.35
ATOM	1411	OD2	ASP	179	30.323	3.605	64.467	1.00	34.72
ATOM	1412	C	ASP	179	30.399	6.357	60.953	1.00	20.84
ATOM	1413	O	ASP	179	31.509	6.146	60.505	1.00	19.20
ATOM	1414	N	ALA	180	29.601	7.293	60.426	1.00	19.98
ATOM	1415	CA	ALA	180	30.052	8.106	59.279	1.00	18.45
ATOM	1416	CB	ALA	180	28.857	8.752	58.604	1.00	17.76
ATOM	1417	C	ALA	180	31.020	9.145	59.822	1.00	18.09
ATOM	1418	O	ALA	180	30.881	9.578	60.960	1.00	18.46
ATOM	1419	N	VAL	181	32.063	9.501	59.124	1.00	17.49
ATOM	1420	CA	VAL	181	33.062	10.462	59.459	1.00	17.25
ATOM	1421	CB	VAL	181	34.320	10.313	58.578	1.00	17.21
ATOM	1422	CG1	VAL	181	35.301	11.466	58.792	1.00	17.56
ATOM	1423	CG2	VAL	181	35.050	9.012	58.805	1.00	17.06
ATOM	1424	C	VAL	181	32.558	11.911	59.223	1.00	18.05
ATOM	1425	O	VAL	181	32.154	12.253	58.113	1.00	16.95
ATOM	1426	N	GLU	182	32.586	12.714	60.268	1.00	17.72
ATOM	1427	CA	GLU	182	32.200	14.126	60.126	1.00	18.58
ATOM	1428	CB	GLU	182	31.974	14.715	61.518	1.00	22.08
ATOM	1429	CG	GLU	182	31.570	16.170	61.478	1.00	26.15
ATOM	1430	CD	GLU	182	31.741	16.841	62.827	1.00	31.27
ATOM	1431	OE1	GLU	182	32.208	16.207	63.810	1.00	32.77
ATOM	1432	OE2	GLU	182	31.553	18.068	62.895	1.00	34.76
ATOM	1433	C	GLU	182	33.434	14.816	59.533	1.00	18.49
ATOM	1434	O	GLU	182	34.509	14.839	60.154	1.00	17.55
ATOM	1435	N	VAL	183	33.323	15.377	58.351	1.00	19.14
ATOM	1436	CA	VAL	183	34.454	16.036	57.698	1.00	20.41

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	1437	CB	VAL	183	34.382	15.826	56.174	1.00	18.55
ATOM	1438	CG1	VAL	183	35.474	16.547	55.414	1.00	17.81
ATOM	1439	CG2	VAL	183	34.544	14.317	55.887	1.00	16.84
ATOM	1440	C	VAL	183	34.624	17.504	58.084	1.00	23.97
ATOM	1441	O	VAL	183	33.925	18.419	57.618	1.00	23.28
ATOM	1442	N	HIS	184	35.657	17.750	58.915	1.00	27.34
ATOM	1443	CA	HIS	184	36.010	19.078	59.381	1.00	30.88
ATOM	1444	CB	HIS	184	36.761	19.018	60.736	1.00	31.42
ATOM	1445	CG	HIS	184	35.950	18.462	61.852	1.00	33.04
ATOM	1446	ND1	HIS	184	36.127	17.192	62.386	1.00	33.48
ATOM	1447	CE1	HIS	184	35.239	16.983	63.324	1.00	33.63
ATOM	1448	NE2	HIS	184	34.472	18.078	63.427	1.00	34.18
ATOM	1449	CD2	HIS	184	34.885	19.009	62.505	1.00	33.72
ATOM	1450	C	HIS	184	36.944	19.774	58.398	1.00	33.03
ATOM	1451	OXT	HIS	184	38.145	19.370	58.369	1.00	34.40
ATOM	1452	O	HIS	184	36.482	20.674	57.663	1.00	34.98
ATOM	1453	O	WAT	185	28.850	21.236	41.157	1.00	7.77
ATOM	1454	O	WAT	186	31.430	6.491	39.145	1.00	5.36
ATOM	1455	O	WAT	187	31.972	20.433	24.682	1.00	19.06
ATOM	1456	O	WAT	188	43.418	17.395	32.297	1.00	7.22
ATOM	1457	O	WAT	189	29.795	9.718	43.035	1.00	13.01
ATOM	1458	O	WAT	190	25.169	14.868	44.564	1.00	7.63
ATOM	1459	O	WAT	191	42.565	13.342	49.566	1.00	12.53
ATOM	1460	O	WAT	192	23.545	16.936	36.967	1.00	11.47
ATOM	1461	O	WAT	193	38.976	27.793	26.907	1.00	19.75
ATOM	1462	O	WAT	194	35.953	1.677	55.506	1.00	8.03
ATOM	1463	O	WAT	195	45.203	4.786	35.591	1.00	19.10
ATOM	1464	O	WAT	196	40.702	22.372	37.469	1.00	5.65
ATOM	1465	O	WAT	197	18.244	27.128	33.934	1.00	9.55
ATOM	1466	O	WAT	198	43.230	2.407	45.385	1.00	14.44
ATOM	1467	O	WAT	199	28.760	15.753	52.327	1.00	6.36
ATOM	1468	O	WAT	200	39.314	16.273	54.340	1.00	10.38
ATOM	1469	O	WAT	201	41.628	6.864	49.085	1.00	13.25
ATOM	1470	O	WAT	202	32.628	8.643	33.259	1.00	14.96
ATOM	1471	O	WAT	203	23.608	15.684	31.276	1.00	11.92
ATOM	1472	O	WAT	204	41.619	27.241	32.862	1.00	12.62
ATOM	1473	O	WAT	205	25.455	16.379	42.062	1.00	9.79
ATOM	1474	O	WAT	206	23.458	25.587	46.689	1.00	9.28
ATOM	1475	O	WAT	207	40.092	2.673	49.703	1.00	21.98
ATOM	1476	O	WAT	208	35.495	30.435	31.702	1.00	9.21

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	1477	O	WAT	209	40.520	4.464	47.917	1.00	17.40
ATOM	1478	O	WAT	210	28.201	9.930	46.793	1.00	14.09
ATOM	1479	O	WAT	211	23.089	19.943	52.306	1.00	14.82
ATOM	1480	O	WAT	212	44.399	21.289	35.915	1.00	13.38
ATOM	1481	O	WAT	213	38.302	11.682	56.310	1.00	13.86
ATOM	1482	O	WAT	214	29.194	31.320	26.877	1.00	14.92
ATOM	1483	O	WAT	215	41.034	0.350	43.151	1.00	8.79
ATOM	1484	O	WAT	216	37.315	5.552	55.980	1.00	15.69
ATOM	1485	O	WAT	217	28.681	5.735	37.072	1.00	27.33
ATOM	1486	O	WAT	218	27.519	26.142	27.532	1.00	20.83
ATOM	1487	O	WAT	220	26.523	16.871	54.153	1.00	7.21
ATOM	1488	O	WAT	221	26.631	8.829	40.556	1.00	13.85
ATOM	1489	O	WAT	222	42.195	14.491	24.181	1.00	18.25
ATOM	1490	O	WAT	223	39.484	2.299	47.684	1.00	17.37
ATOM	1491	O	WAT	224	42.696	5.852	33.808	1.00	21.32
ATOM	1492	O	WAT	225	21.738	21.298	24.368	1.00	34.50
ATOM	1493	O	WAT	226	22.987	10.820	52.989	1.00	14.83
ATOM	1494	O	WAT	227	46.793	19.037	41.919	1.00	17.41
ATOM	1495	O	WAT	228	50.134	12.914	25.200	1.00	13.49
ATOM	1496	O	WAT	229	34.941	32.358	33.918	1.00	10.04
ATOM	1497	O	WAT	230	29.840	4.973	57.907	1.00	13.19
ATOM	1498	O	WAT	231	41.476	32.535	41.932	1.00	16.82
ATOM	1499	O	WAT	233	47.577	10.560	24.957	1.00	14.85
ATOM	1500	O	WAT	234	31.423	7.923	35.851	1.00	18.25
ATOM	1501	O	WAT	235	24.429	27.131	29.298	1.00	20.86
ATOM	1502	O	WAT	236	45.316	2.958	43.842	1.00	16.57
ATOM	1503	O	WAT	237	46.300	14.369	48.285	1.00	15.62
ATOM	1504	O	WAT	238	22.551	21.212	56.437	1.00	20.75
ATOM	1505	O	WAT	240	42.496	7.817	57.030	1.00	36.21
ATOM	1506	O	WAT	241	29.753	7.840	45.086	1.00	20.48
ATOM	1507	O	WAT	242	44.157	18.020	35.284	1.00	15.10
ATOM	1508	O	WAT	243	32.571	28.209	41.063	1.00	26.82
ATOM	1509	O	WAT	244	29.928	3.636	51.745	1.00	17.99
ATOM	1510	O	WAT	245	17.606	26.422	41.913	1.00	14.25
ATOM	1511	O	WAT	246	20.589	12.991	55.488	1.00	19.81
ATOM	1512	O	WAT	247	39.341	29.548	29.158	1.00	18.35
ATOM	1513	O	WAT	248	17.156	16.295	61.445	1.00	12.69
ATOM	1514	O	WAT	249	24.354	14.243	33.242	1.00	12.22
ATOM	1515	O	WAT	250	32.830	14.766	20.087	1.00	25.25
ATOM	1516	O	WAT	251	16.815	19.536	36.675	1.00	15.62

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	1517	O	WAT	252	28.441	34.415	30.350	1.00	14.51
ATOM	1518	O	WAT	253	26.031	8.747	44.300	1.00	20.25
ATOM	1519	O	WAT	254	43.077	16.183	18.629	1.00	31.67
ATOM	1520	O	WAT	256	33.197	19.064	19.853	1.00	24.22
ATOM	1521	O	WAT	257	30.278	20.250	16.867	1.00	42.28
ATOM	1522	O	WAT	258	20.798	17.479	26.186	1.00	29.53
ATOM	1523	O	WAT	259	35.416	13.350	21.607	1.00	22.56
ATOM	1524	O	WAT	260	35.637	44.109	41.691	1.00	21.90
ATOM	1525	O	WAT	261	24.100	18.625	43.187	1.00	8.00
ATOM	1526	O	WAT	263	22.843	12.530	27.491	1.00	22.94
ATOM	1527	O	WAT	264	44.179	24.395	43.693	1.00	23.48
ATOM	1528	O	WAT	265	18.860	10.472	42.233	1.00	22.82
ATOM	1529	O	WAT	266	16.026	26.688	39.851	1.00	14.46
ATOM	1530	O	WAT	267	26.345	14.750	24.426	1.00	23.54
ATOM	1531	O	WAT	268	37.901	14.303	60.873	1.00	57.94
ATOM	1532	O	WAT	269	23.911	8.885	51.213	1.00	19.17
ATOM	1533	O	WAT	270	25.088	18.293	25.334	1.00	21.16
ATOM	1534	O	WAT	271	32.345	12.423	22.061	1.00	26.85
ATOM	1535	O	WAT	272	29.849	8.405	23.646	1.00	22.55
ATOM	1536	O	WAT	273	38.933	19.380	16.508	1.00	29.99
ATOM	1537	O	WAT	274	28.930	6.191	30.272	1.00	30.24
ATOM	1538	O	WAT	277	51.699	18.896	51.858	1.00	26.44
ATOM	1539	O	WAT	278	26.732	24.016	51.882	1.00	20.15
ATOM	1540	O	WAT	280	35.901	30.991	27.045	1.00	31.15
ATOM	1541	O	WAT	281	34.878	34.657	45.573	1.00	23.59
ATOM	1542	O	WAT	282	22.582	24.196	49.931	1.00	17.52
ATOM	1543	O	WAT	283	25.665	18.480	61.477	1.00	22.72
ATOM	1544	O	WAT	285	16.617	23.741	53.679	1.00	22.92
ATOM	1545	O	WAT	286	27.425	5.238	57.616	1.00	28.57
ATOM	1546	O	WAT	287	24.194	17.156	62.543	1.00	22.92
ATOM	1547	O	WAT	288	43.605	13.871	55.205	1.00	47.34
ATOM	1548	O	WAT	289	14.252	10.820	52.850	1.00	28.43
ATOM	1549	O	WAT	291	29.445	0.878	44.981	1.00	19.69
ATOM	1550	O	WAT	292	33.986	13.974	64.333	1.00	37.04
ATOM	1551	O	WAT	293	41.717	34.544	35.754	1.00	26.74
ATOM	1552	O	WAT	294	44.822	15.305	22.321	1.00	16.03
ATOM	1553	O	WAT	295	36.295	31.861	47.655	1.00	26.65
ATOM	1554	O	WAT	296	42.599	28.766	43.606	1.00	26.10
ATOM	1555	O	WAT	297	39.805	5.761	18.396	1.00	41.39
ATOM	1556	O	WAT	298	13.973	17.827	35.310	1.00	54.73

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	1557	O	WAT	299	27.996	7.316	26.790	1.00	18.08
ATOM	1558	O	WAT	300	42.886	21.511	50.516	1.00	18.76
ATOM	1559	O	WAT	303	49.197	25.130	46.385	1.00	34.63
ATOM	1560	O	WAT	304	30.514	20.096	22.934	1.00	26.25
ATOM	1561	O	WAT	305	16.070	11.629	32.114	1.00	33.09
ATOM	1562	O	WAT	307	45.009	9.505	49.911	1.00	38.13
ATOM	1563	O	WAT	308	19.596	10.468	29.457	1.00	17.29
ATOM	1564	O	WAT	309	15.205	14.450	44.995	1.00	14.06
ATOM	1565	O	WAT	310	29.356	16.954	20.232	1.00	31.55
ATOM	1566	O	WAT	311	24.108	38.264	35.844	1.00	39.11
ATOM	1567	O	WAT	312	35.407	6.361	25.290	1.00	30.83
ATOM	1568	O	WAT	313	39.712	31.481	26.164	1.00	59.55
ATOM	1569	O	WAT	314	46.008	26.765	46.643	1.00	24.46
ATOM	1570	O	WAT	315	31.206	32.756	27.472	1.00	25.26
ATOM	1571	O	WAT	316	50.563	22.574	47.365	1.00	33.15
ATOM	1572	O	WAT	317	44.191	6.963	54.611	1.00	37.60
ATOM	1573	O	WAT	318	25.966	3.136	59.271	1.00	35.51
ATOM	1574	O	WAT	319	37.521	28.687	19.179	1.00	42.82
ATOM	1575	O	WAT	320	37.860	6.732	23.019	1.00	29.39
ATOM	1576	O	WAT	321	16.404	30.148	38.616	1.00	44.90
ATOM	1577	O	WAT	322	20.948	10.666	55.483	1.00	20.70
ATOM	1578	O	WAT	323	42.010	40.095	40.065	1.00	30.74
ATOM	1579	O	WAT	324	34.974	43.535	31.498	1.00	33.73
ATOM	1580	O	WAT	325	36.339	21.393	17.438	1.00	22.90
ATOM	1581	O	WAT	326	22.573	26.604	27.035	1.00	25.45
ATOM	1582	O	WAT	327	43.925	1.275	33.700	1.00	31.52
ATOM	1583	O	WAT	328	44.055	25.497	31.799	1.00	25.75
ATOM	1584	O	WAT	329	21.385	6.303	61.996	1.00	33.54
ATOM	1585	O	WAT	330	29.459	11.771	63.481	1.00	30.61
ATOM	1586	O	WAT	331	44.458	29.701	35.168	1.00	21.73
ATOM	1587	O	WAT	332	44.874	3.401	28.884	1.00	21.60
ATOM	1588	O	WAT	333	35.791	46.126	38.798	1.00	31.81
ATOM	1589	O	WAT	335	42.315	35.196	45.915	1.00	81.46
ATOM	1590	O	WAT	336	31.457	36.447	45.501	1.00	48.90
ATOM	1591	O	WAT	337	21.963	8.289	49.003	1.00	25.78
ATOM	1592	O	WAT	338	46.389	28.795	37.209	1.00	25.28
ATOM	1593	O	WAT	339	24.612	30.116	24.354	1.00	52.56
ATOM	1594	O	WAT	340	32.083	2.650	30.885	1.00	67.46
ATOM	1595	O	WAT	341	44.830	28.999	40.931	1.00	47.88
ATOM	1596	O	WAT	342	30.337	12.782	23.955	1.00	18.21

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	1597	O	WAT	343	28.938	3.896	35.075	1.00	33.18
ATOM	1598	O	WAT	344	14.617	18.243	39.459	1.00	29.61
ATOM	1599	O	WAT	345	24.634	22.916	24.622	1.00	27.73
ATOM	1600	O	WAT	346	39.434	34.582	32.483	1.00	20.28
ATOM	1601	O	WAT	347	12.161	23.144	40.518	1.00	61.26
ATOM	1602	O	WAT	348	27.481	2.007	50.279	1.00	79.56
ATOM	1603	O	WAT	349	42.979	34.755	39.897	1.00	44.74
ATOM	1604	O	WAT	350	28.778	41.078	42.112	1.00	28.20
ATOM	1605	O	WAT	351	17.300	10.548	37.874	1.00	43.80
ATOM	1606	O	WAT	352	19.099	8.296	59.238	1.00	40.38
ATOM	1607	O	WAT	353	27.220	31.276	48.083	1.00	40.23
ATOM	1608	O	WAT	354	25.981	34.775	41.644	1.00	40.74
ATOM	1609	O	WAT	355	27.143	6.951	48.473	1.00	25.01
ATOM	1610	O	WAT	356	38.151	11.528	18.954	1.00	25.07
ATOM	1611	O	WAT	357	19.762	7.319	56.021	1.00	25.55
ATOM	1612	O	WAT	358	28.144	1.582	55.375	1.00	89.67
ATOM	1613	O	WAT	360	27.638	16.644	62.799	1.00	23.18
ATOM	1614	O	WAT	361	14.684	31.678	44.174	1.00	71.66
ATOM	1615	O	WAT	362	15.650	11.558	66.663	1.00	64.23
ATOM	1616	O	WAT	363	15.237	18.359	54.178	1.00	39.41
ATOM	1617	O	WAT	364	43.172	16.847	51.474	1.00	22.97
ATOM	1618	O	WAT	365	18.986	26.729	27.844	1.00	48.99
ATOM	1619	O	WAT	366	27.139	19.402	23.399	1.00	29.96
ATOM	1620	O	WAT	367	45.600	0.114	38.791	1.00	74.35
ATOM	1621	O	WAT	369	19.987	11.960	57.958	1.00	16.62
ATOM	1622	O	WAT	372	27.335	27.231	54.352	1.00	40.25
ATOM	1623	O	WAT	373	15.884	15.171	31.990	1.00	16.33
ATOM	1624	O	WAT	374	15.330	24.772	50.039	1.00	32.03
ATOM	1625	O	WAT	377	43.724	3.843	52.380	1.00	65.10
ATOM	1626	O	WAT	378	38.825	38.327	52.464	1.00	49.54
ATOM	1627	O	WAT	379	46.669	23.629	33.133	1.00	28.01
ATOM	1628	O	WAT	380	25.700	12.197	66.584	1.00	89.69
ATOM	1629	O	WAT	381	16.946	9.817	50.702	1.00	39.01
ATOM	1630	O	WAT	382	28.300	9.517	63.491	1.00	33.60
ATOM	1631	O	WAT	384	46.564	10.837	53.832	1.00	46.92
ATOM	1632	O	WAT	385	19.884	8.624	51.494	1.00	27.80
ATOM	1633	O	WAT	387	40.902	2.984	29.363	1.00	31.27
ATOM	1634	O	WAT	391	34.316	2.463	62.378	1.00	58.47
ATOM	1635	O	WAT	392	33.435	11.543	52.204	1.00	30.98
ATOM	1636	O	WAT	393	31.770	25.813	26.248	1.00	27.06

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	1637	O	WAT	400	29.567	21.566	48.768	1.00	15.75
ATOM	1638	O	WAT	402	48.664	8.376	47.162	1.00	18.07
ATOM	1639	O	WAT	403	27.502	36.401	36.418	1.00	21.54
ATOM	1640	O	WAT	404	38.545	3.037	55.400	1.00	13.22
ATOM	1641	O	WAT	405	31.109	23.890	44.564	1.00	12.95
ATOM	1642	O	WAT	406	37.990	6.814	28.956	1.00	20.51
ATOM	1643	O	WAT	407	23.258	29.488	41.877	1.00	11.41
ATOM	1644	O	WAT	409	38.433	6.626	31.944	1.00	19.15
ATOM	1645	O	WAT	410	31.295	21.118	43.998	1.00	14.11
ATOM	1646	O	WAT	411	29.526	7.658	41.193	1.00	14.42
ATOM	1647	O	WAT	412	47.253	15.532	34.182	1.00	15.59
ATOM	1648	O	WAT	413	32.025	22.355	49.225	1.00	22.54
ATOM	1649	O	WAT	414	35.003	0.189	57.857	1.00	17.18
ATOM	1650	O	WAT	415	38.803	38.578	33.800	1.00	50.11
ATOM	1651	O	WAT	416	31.617	3.615	39.556	1.00	15.08
ATOM	1652	O	WAT	417	41.233	19.520	51.473	1.00	26.94
ATOM	1653	O	WAT	418	34.336	27.496	25.242	1.00	32.64
ATOM	1654	O	WAT	419	31.486	2.145	58.952	1.00	26.96
ATOM	1655	O	WAT	420	20.483	8.464	45.003	1.00	39.84
ATOM	1656	O	WAT	421	38.402	6.719	60.710	1.00	53.78
ATOM	1657	O	WAT	422	17.225	14.988	64.662	1.00	27.63
ATOM	1658	O	WAT	423	29.858	4.786	43.647	1.00	25.15
ATOM	1659	O	WAT	424	30.773	22.384	54.282	1.00	36.55
ATOM	1660	O	WAT	425	38.526	14.414	56.721	1.00	20.85
ATOM	1661	O	WAT	426	30.456	20.512	46.952	1.00	19.94
ATOM	1662	O	WAT	427	22.093	34.199	38.603	1.00	30.42
ATOM	1663	O	WAT	428	29.003	23.510	42.193	1.00	14.64
ATOM	1664	O	WAT	430	24.931	30.471	52.337	1.00	30.16
ATOM	1665	O	WAT	431	48.705	28.493	42.035	1.00	55.68
ATOM	1666	O	WAT	432	39.117	4.219	32.847	1.00	25.71
ATOM	1667	O	WAT	433	26.609	27.683	58.327	1.00	27.50
ATOM	1668	O	WAT	434	39.186	-0.478	36.174	1.00	49.55
ATOM	1669	O	WAT	435	41.271	4.828	21.864	1.00	39.72
ATOM	1670	O	WAT	436	41.092	33.182	29.047	1.00	32.94
ATOM	1671	O	WAT	437	15.296	21.832	45.786	1.00	40.79
ATOM	1672	O	WAT	438	28.338	42.926	45.181	1.00	54.46
ATOM	1673	O	WAT	439	18.910	32.039	47.096	1.00	34.92
ATOM	1674	O	WAT	440	20.737	30.240	33.890	1.00	27.30
ATOM	1675	O	WAT	441	39.566	2.311	52.603	1.00	9.84
ATOM	1676	O	WAT	442	26.307	7.449	29.241	1.00	24.87

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	1677	O	WAT	443	33.345	6.388	32.193	1.00	25.75
ATOM	1678	O	WAT	444	31.294	5.444	34.030	1.00	30.09
ATOM	1679	O	WAT	445	28.477	5.556	33.091	1.00	33.90
ATOM	1680	O	WAT	446	35.818	5.354	27.499	1.00	34.01
ATOM	1681	O	WAT	447	38.643	6.449	25.935	1.00	36.56
ATOM	1682	O	WAT	448	32.925	5.503	23.694	1.00	34.87
ATOM	1683	O	WAT	449	36.725	28.997	25.274	1.00	30.86
ATOM	1684	O	WAT	450	33.363	29.455	26.675	1.00	37.40
ATOM	1685	O	WAT	451	41.451	27.420	25.703	1.00	33.62
ATOM	1686	O	WAT	452	29.410	26.542	26.305	1.00	29.99
ATOM	1687	O	WAT	453	36.755	35.395	27.932	1.00	31.87
ATOM	1688	O	WAT	454	38.358	33.650	29.807	1.00	27.03
ATOM	1689	O	WAT	455	37.465	31.045	29.786	1.00	24.00
ATOM	1690	O	WAT	456	36.203	38.857	29.055	1.00	33.74
ATOM	1691	O	WAT	457	43.139	26.818	23.216	1.00	42.86
ATOM	1692	O	WAT	458	44.010	27.925	26.702	1.00	35.47
ATOM	1693	O	WAT	459	42.654	24.489	23.829	1.00	36.86
ATOM	1694	O	WAT	460	41.901	30.150	29.907	1.00	28.79
ATOM	1695	O	WAT	461	26.772	28.402	27.845	1.00	24.54
ATOM	1696	O	WAT	462	26.549	25.016	24.992	1.00	30.41
ATOM	1697	O	WAT	463	24.198	25.675	25.291	1.00	29.34
ATOM	1698	O	WAT	464	18.389	23.209	26.099	1.00	27.72
ATOM	1699	O	WAT	465	15.792	17.751	27.506	1.00	35.38
ATOM	1700	O	WAT	466	18.177	19.068	27.187	1.00	29.61
ATOM	1701	O	WAT	467	20.277	34.110	40.402	1.00	39.33
ATOM	1702	O	WAT	468	22.420	34.685	35.945	1.00	32.47
ATOM	1703	O	WAT	469	25.586	36.936	38.120	1.00	30.14
ATOM	1704	O	WAT	470	22.975	32.962	41.300	1.00	37.30
ATOM	1705	O	WAT	471	22.668	19.271	25.898	1.00	29.84
ATOM	1706	O	WAT	472	18.891	9.006	33.972	1.00	36.50
ATOM	1707	O	WAT	473	24.180	8.334	27.833	1.00	29.82
ATOM	1708	O	WAT	474	26.583	4.932	30.103	1.00	31.47
ATOM	1709	O	WAT	475	35.276	12.918	19.062	1.00	29.07
ATOM	1710	O	WAT	476	37.941	14.051	18.038	1.00	30.43
ATOM	1711	O	WAT	477	38.446	16.323	16.217	1.00	33.99
ATOM	1712	O	WAT	478	38.163	8.369	18.377	1.00	28.75
ATOM	1713	O	WAT	479	42.854	7.090	21.196	1.00	35.78
ATOM	1714	O	WAT	480	43.719	8.314	25.189	1.00	18.37
ATOM	1715	O	WAT	481	44.810	8.599	19.951	1.00	33.64
ATOM	1716	O	WAT	482	47.966	7.671	21.852	1.00	31.71

TABLE 1: Structure Coordinates for *S. aureus* pdf

ATOM	1717	O	WAT	483	45.820	13.136	19.737	1.00	32.03
ATOM	1718	O	WAT	484	31.751	17.094	18.635	1.00	30.24
ATOM	1719	O	WAT	485	27.993	14.973	20.979	1.00	33.51
ATOM	1720	O	WAT	486	26.220	11.398	22.499	1.00	33.95
ATOM	1721	O	WAT	487	28.510	14.814	17.996	1.00	35.70
ATOM	1722	O	WAT	488	33.549	20.609	17.456	1.00	30.90
ATOM	1723	O	WAT	489	27.960	13.392	23.087	1.00	26.06
ATOM	1724	O	WAT	490	40.175	20.917	14.980	1.00	37.89
ATOM	1725	ZN	Zn	500	26.949	20.605	41.894	1.00	12.48
END									